European Journal of Operational Research 000 (2016) 1–19

Contents lists available at ScienceDirect

European Journal of Operational Research

journal homepage: www.elsevier.com/locate/ejor

Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis

Miłosz Kadziński[a,*], Marco Cinelli[b,c], Krzysztof Ciomek[a], Stuart R. Coles[b], Mallikarjuna N. Nadagouda[d], Rajender S. Varma[e], Kerry Kirwan[b]

[a] Institute of Computing Science, Poznań University of Technology, Piotrowo 2, Poznań 60-965, Poland
[b] WMG, International Manufacturing Centre, University of Warwick, Coventry, CV4 7AL, UK
[c] Institute of Advanced Study, Millburn House, University of Warwick Science Park, Coventry, CV4 7HS, UK
[d] ORD, NRMRL, WSWRD, WQMB, U.S. Environmental Protection Agency, Cincinnati, OH, 45268, USA
[e] Sustainable Technology Division, National Risk Management Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH, 45268, USA

ARTICLE INFO

Article history:
Received 1 January 2016
Accepted 10 October 2016
Available online xxx

Keywords:
Multiple criteria analysis
Green chemistry
Silver nanoparticles
Sustainability
Ordinal classification

ABSTRACT

Nanomaterials (materials at the nanoscale, 10^{-9} meters) are extensively used in several industry sectors due to the improved properties they empower commercial products with. There is a pressing need to produce these materials more sustainably. This paper proposes a Multiple Criteria Decision Aiding (MCDA) approach to assess the implementation of green chemistry principles as applied to the protocols for nanoparticles synthesis. In the presence of multiple green and environmentally oriented criteria, decision aiding is performed with a synergy of ordinal regression methods; preference information in the form of desired assignment for a subset of reference protocols is accepted. The classification models, indirectly derived from such information, are composed of an additive value function and a vector of thresholds separating the pre-defined and ordered classes. The method delivers a single representative model that is used to assess the relative importance of the criteria, identify the possible gains with improvement of the protocol's evaluations and classify the non-reference protocols. Such precise recommendation is validated against the outcomes of robustness analysis exploiting the sets of all classification models compatible with all maximal subsets of consistent assignment examples. The introduced approach is used with real-world data concerning silver nanoparticles. It is proven to effectively resolve inconsistency in the assignment examples, tolerate ordinal and cardinal measurement scales, differentiate between inter- and intra-criteria attractiveness and deliver easily interpretable scores and class assignments. This work thoroughly discusses the learning insights that MCDA provided during the co-constructive development of the classification model.

1. Introduction

Nanotechnology is the manipulation of matter at the nanoscale (one billionth of a meter, 10^{-9} meters) to produce materials (i.e., nanomaterials) with enhanced performances. During the last decade it has experienced a sizeable development (Iavicoli, Leso, Ricciardi, Hodson, & Hoover, 2014; Shapira & Youtie, 2012; 2015). Plethora of nanotechnology applications are emerging in several industrial sectors (e.g., biomedical, cosmetics, electronic, energy, engineering, textile, packaging, food and drinks) and due to its pervasive nature there is a pressing need for assessing the implications of this fast-pace development on the environment, economy and society (Iavicoli et al., 2014; Karn & Wong, 2013; Shapira & Youtie, 2015). Achieving this objective involves the use of multiple assessment criteria, which represents a complex decision problem with conflicting viewpoints. This paper contributes to this area by proposing a Multiple Criteria Decision Aiding (MCDA) approach to support environmentally sustainable synthesis of nanomaterials.

The synthesis stage has been a premier focus of the research on nanomaterials development, as it is the fundamental step where the design of the product is defined, the functionality is shaped, the reliability empowered and an important contribution to the sustainability implications is determined (Dahl, Maddux, & Hutchison, 2007; Hutchison, 2008; Patete et al., 2011). In order to guarantee a responsible supply of nanomaterials many synthesis processes have been developed to take their sustainability impacts into consideration. In this way, the principles of green chemistry (Anastas & Warner, 1998) and engineering (Anastas & Zimmerman,

* Corresponding author. Fax: +48 61 8771 525.
E-mail address: milosz.kadzinski@cs.put.poznan.pl (M. Kadziński).

http://dx.doi.org/10.1016/j.ejor.2016.10.019
0377-2217/

2003) started being integrated into this life-cycle stage (Anastas & Warner, 1998; Eckelman, Zimmerman, & Anastas, 2008; Gilbertson, Zimmerman, Plata, Hutchison, & Anastas, 2015; Hutchison, 2008; Patete et al., 2011).

Indeed, these innovative approaches account for such principles by increasing energy efficiency, using renewable and less hazardous materials, increasing speed reactions and ensuring safer operating conditions (Dahl et al., 2007; Gawande, Shelke, Zboril, & Varma, 2014; Nadagouda et al., 2014; Patete et al., 2011; Varma, 2013; 2014; Virkutyte & Varma, 2013). At the same time, they succeed to produce nanoparticles with desired uniform size and shape. To assess the implementation of green chemistry principles by the synthesis protocols, it is necessary to account for a number of evaluation criteria in an integrated manner. This suggests the appropriateness of using MCDA methods whose role is to provide and justify decision recommendations in the presence of multiple conflicting points of view. More specifically, there is currently a demand for classification methods that can be used to assign a preference-oriented performance class to the synthesis processes for nanomaterials, showing how "green" they actually are (Bergeson, 2013; Gilbertson et al., 2015; Mata, Martins, Costa, & Sikdar, 2015).

This paper proposes an MCDA model for classifying synthesis protocols into a set of pre-defined and ordered green chemistry-based classes and exemplifies its application for the silver nanoparticles, particles of silver at the nanoscale. The methodology that supported the model development implements the paradigm of Ordinal Regression (ORDREG) (Jacquet-Lagrèze & Siskos, 2001) (or preference disaggregation, Doumpos & Zopounidis, 2011) by inferring compatible models composed of an additive value function and extrapolating class thresholds from the assignment examples provided by nanotechnology experts. Then, these models are used to suggest an assignment for the remaining protocols. This work has been conceived as a complementary strategy to the one advanced by Cinelli et al. (2015) where Dominance-based Rough Set Approach (DRSA) (Błaszczyński, Słowiński, & Szelag, 2011; Greco, Matarazzo, & Słowiński, 2001) was employed to the same problem and provided a classification model based on decision rules.

The proposed integrated approach combines a few procedures whose properties were found to be useful to support sustainability assessment and it contributes to the preference learning process that is hallmark of MCDA. First, the method is able to integrate the expert knowledge, being usable even in case the provided preference information is inconsistent. This is achieved by automatic identification of all maximal sets of consistent assignment examples. Second, it effectively deals with both qualitative and quantitative criteria by applying general value functions. Third, the approach constructs a representative model that indicates which factors are most important for the classification. This model differentiates also the intra-criterion attractiveness with possibly non-convex or non-concave shape of a marginal value function. Fourth, it quantifies how green the synthesis protocols are by performing aggregation of alternatives' evaluation on all considered criteria. Fifth, thanks to the applied threshold-based classification procedure, the underlying decision aiding process is intuitive and transparent even for the non-experts in MCDA field. Sixth, the delivered recommendation is easily interpretable and justifiable due to the decomposition of overall values into marginal ones. The latter provide thorough insight into each protocol's strengths and weaknesses. Finally, the method builds on the synergy of ORDREG methods. In this way, it provides means for verifying the certainty of an assignment suggested by a single representative model against the outcomes of Robust Ordinal Regression (ROR) (Corrente, Greco, Kadziński, & Słowiński, 2013; Greco, Mousseau, & Słowiński, 2008) and Stochastic Ordinal Regression (SOR) (Kadziński & Tervonen, 2013a; 2013b) derived from all classification models compatible with all maximal sets of consistent assignment examples. ROR indicates which assignments are possible using Linear Programing (LP) techniques, whereas SOR estimates the probability of such possibility with Monte Carlo simulation. In this way, the constructed recommendation can be deemed robust.

By exhibiting all these features when reporting results of the case study, the paper aims to show that the proposed method is able to effectively support not only the development and assessment of nanoparticle synthesis, but also other decision making contexts oriented toward sustainability. Overall, this paper has the following objectives:

- Propose (Section 2) and test (Section 3) a new methodology based on ORDREG for classification of synthesis processes of silver nanoparticles based on green chemistry principles implementation.
- Highlight the practical learning derived from the use of MCDA in this applied research. Throughout the paper, we illustrate how MCDA is a ductile process that allows structuring a complex and undefined problem, define the alternatives to be assessed, the evaluation parameters and shape a robust decision support model.

2. Methodology

An important issue in nanotechnology is the development of production processes for nanomaterials, since they have a pivotal role in determining the properties of the ensuing product, its reliability and the impacts that it can have from a sustainability perspective (Duan, Wang, & Li, 2015; Sengul, Theis, & Ghosh, 2008). The processes that received major attention in the last decade are those performed with more responsible, green and sustainable approaches, integrating the principles of green chemistry and green engineering in the nanosynthesis practice (Dahl et al., 2007; Duan et al., 2015; Gilbertson et al., 2015; Mata et al., 2015; Nadagouda et al., 2014; Patete et al., 2011; Varma, 2013; 2014).

So far bacteria, fungi, plants, plants extracts, yeasts and algae have been employed to produce nanomaterials, receiving the label of bio-inspired reduction approaches and employing several principles of green chemistry, including renewable materials use, synthesis at ambient temperature and pressure as well as safe processing conditions (Das & Marsili, 2011; Korbekandi, Iravani, & Abbasi, 2009; Stark, Stoessel, Wohlleben, & Hafner, 2015; Virkutyte & Varma, 2013). Understanding and assessing how "green" these bio-inspired processes are is hampered by several challenges, including (i) the need to account for impacts criteria of different type (e.g., quantitative, qualitative, fuzzy) (Eason, Meyer, Curran, & Upadhyayula, 2011; Mata et al., 2015; Naidu, 2012), (ii) high uncertainty in input dataset (Hischier, 2014; Mata et al., 2015; Meyer & Upadhyayula, 2014), and (iii) limited capacities of conventional tools to provide a comprehensive and justifiable performance of each process (Bates, Larkin, Keisler, and Linkov, 2015; Eason et al., 2011; Tsang, Bates, Madison & Linkov, 2014).

MCDA has been specifically developed to tackle these types of challenges (Cinelli, Coles, & Kirwan, 2014; Munda, 2005), especially in cases where the problems are ill-defined, which is another peculiar characteristic of sustainability assessment of nanosynthesis. Such problem framing justified the use of MCDA in the case study, to develop a classification model for the performance evaluation of synthesis of nanomaterials with respect to implementation of the green-chemistry principles. The research objective was achieved through the application of the MCDA process, tailored to this decision making problem. Fig. 1 summarizes the procedure. Its phases are described in detail in the following sections.

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

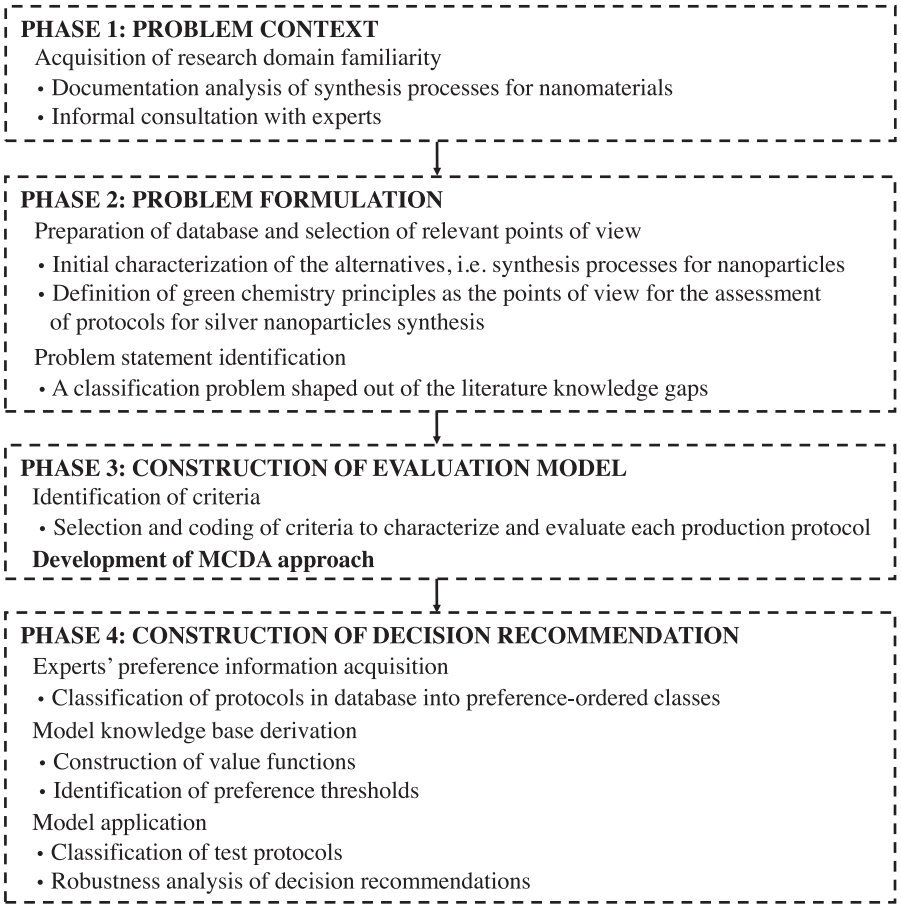

Fig. 1. List and links between MCDA process phases and steps in experts knowledge elicitation for the construction of classification model (adapted from Hoffman, Shadbolt, Burton, & Klein, 1995; Tsoukiás, 2007).

2.1. Phase 1: problem context

A broad literature review of production processes for nanomaterials was conducted to define the context of the research. It confirmed that bio-inspired synthesis routes are receiving wide interest because of their potentials of implementing green chemistry principles (Changseok et al., 2013; Cinelli et al., 2015; Dahl et al., 2007; Duan et al., 2015; Dubey, Lahtinen, & Sillanpaa, 2010; Hebbalalu, Lalley, Nadagouda, & Varma, 2013; Hyeon, Manna, & Wong, 2015; Karn, 2008; Karn & Wong, 2013; Kavitha et al., 2013; Kaviya, Santhanalakshmi, Viswanathan, Muthumary, & Srinivasan, 2011; Kou, Bennett-Stamper, & Varma, 2013; Kou & Varma, 2012; Luque, 2013; Matus, Hutchinson, Peoples, Rung, & Tanguay, 2011; Patete et al., 2011; Pati, Sean, & Vikeseland, 2014; Senjen, 2009; Varma, 2014; Virkutyte & Varma, 2013). In-depth understanding of the problem situation was enhanced by the collaboration with two experts (the DMs) in the area of nanotechnology, who took part in the whole decision aiding process. The major limitations that emerged during this initial scoping phase were that the domain of "greenness" assessment of nanosynthesis is ill-defined, due to the paucity of (i) understanding of the optimal conditions and equipment requirements for large scale bio-inspired processes, (ii) quantitative data to run complete life cycle assessments, and (iii) easily accessible decision support models that can help chemists and engineers conducting screening level assessments with heterogeneous (e.g., qualitative, quantitative, fuzzy) and uncertain information to define how green nanosynthesis processes are (Duan et al., 2015; Eason et al., 2011; Hyeon et al., 2015; Linkov, Anklam, Collier, DiMase, & Renn, 2014; Linkov & Moberg, 2011; Mata et al., 2015; Upreti, Dhingra, Naidu, Atuahene, & Sawhney, 2015). The latter research gap appeared as a crucial one to be filled since synthesis processes for nanomaterials keep emerging and there is a pressing necessity for tools that can help their responsible governance (Bates et al., 2015; Cinelli et al., 2015; Linkov, Kurth, Hristozov, & Keisler, 2015; Sadik, Karn, & Keller, 2014; Subramanian et al., 2015). This paper is concerned with such challenge and the MCDA process was shaped in order to provide a useful contribution in the area.

2.2. Phase 2: problem formulation

Problem formulation began with the identification of the alternatives. These were defined as "silver nanoparticle synthesis protocols based on bottom-up approaches that use reducing and capping agents to convert a silver salt to silver nanoparticles". In less technical terms, the reducing agents in these protocols have the capacity of turning the silver salt (i.e., precursor) into silver nanoparticles, while the capping agents protect the nanoparticles from agglomeration. Overall, the collaboration between the analysts and the DMs in our study led to defining a structure dataset of 53 synthesis protocols.

Two main reasons justified the choice for the alternatives: (i) a wide spectrum of synthesis processes have been advanced for the production of silver nanoparticles through a variety of conventional as well as bio-inspired reduction strategies, providing the background for the development of a database of comparable synthesis protocols using sustainability-oriented criteria for this nanomaterial (Changseok et al., 2013; Dahl et al., 2007; Duan et al., 2015; Dubey et al., 2010; Hebbalalu et al., 2013; Karn, 2008;

Table 1
Green chemistry principles – points of view for the assessment of alternatives in the case study (Anastas & Warner, 1998).

	Principle	Description
1	Prevention	Production of waste should be minimized rather than treated after it is formed
2	Atom economy	Use raw materials as efficiently as possible to incorporate them into the final product
3	Less hazardous chemical synthesis	Develop synthetic processes that employ and yield substances as benign as possible
4	Designing safer chemicals	Reduce toxicity of the desired product while maintaining its functionality
5	Safer solvents and auxiliaries	Use harmless auxiliaries in the lowest unavoidable amount
6	Design for energy efficiency	Aim for production processes performed at room pressure and temperature
7	Use of renewable feedstocks	Employ materials that are renewable rather than exhaustible
8	Reduce derivatives	Limit as much as possible the need of derivatives (e.g., blocking groups, transitional modifications)
9	Catalysis	Use reagents that are catalytic rather than stoichiometric
10	Design for degradation	Develop products that turn into hazardless compounds once their function has been performed
11	Real-time analysis for pollution prevention	Adopt real-time and in-process supervision to prevent formation of hazardous materials
12	Inherently safer chemistry for accident prevention	Choose substances that can minimize accidents potentials of the reaction

Karn & Wong, 2013; Kavitha et al., 2013; Kaviya et al., 2011; Kou et al., 2013; Kou & Varma, 2012; Luque, 2013; Matus et al., 2011; Patete et al., 2011; Pati et al., 2014; Senjen, 2009; Varma, 2014; Virkutyte & Varma, 2013); (ii) various applications are enabled and envisioned by silver nanoparticles, such as antimicrobial products, biosensors and composite fibers (Hebbalalu et al., 2013; Korbekandi et al., 2009; Stark et al., 2015; Virkutyte & Varma, 2013).

Green chemistry principles (see Table 1) were selected as the main points of view (PoVs) to characterize and assess the synthesis protocols since they represent the premier strategies to make a process "green" (Anastas & Warner, 1998; Duan et al., 2015). A wide variety of production processes for silver nanoparticles have been advanced to integrate sustainability principles in the synthesis step of nanomaterials as mentioned in the introduction and in the relevant literature (Dahl et al., 2007; Gawande et al., 2014; Nadagouda et al., 2014; Patete et al., 2011; Varma, 2013; 2014; Virkutyte & Varma, 2013). However, most of the studies focus on the individual proposition of a synthesis protocol and not on comparing them to fill research gaps advanced by well-regarded practitioners and organizations in the area (Bergeson, 2013; Dahl et al., 2007; Hutchison, 2008; Karn & Wong, 2013; Luque, 2013; Matus et al., 2011), being:

- identification of the specific reasons for which some protocols perform better than others from a green chemistry perspective;
- assessment of the implementation of green chemistry principles in nanosynthesis processes in the form of a performance class (e.g., "green" nano).

From a decision making viewpoint, these aims correspond to a specific classification problem. Considering that MCDA has been specifically developed to handle comparisons and provide classifications (among other types of decision recommendation) of competing alternatives, it was selected here to advance the solutions. Precisely, the case study is oriented towards the assignment of the protocols to five pre-defined and preference ordered classes with C_5 and C_1 being, respectively, the best class and the worst class. The interpretation of these classes refers to the comprehensive (C_5), considerable (C_4), partial (C_3), limited (C_2) and very marginal (C_1) adoption of green chemistry principles, satisfaction of quality requirements and regard for environmental implications.

2.3. Phase 3: evaluation model

The PoVs identified at the problem structuring phase were made operational during the third step of the MCDA process, namely the construction of the evaluation model. Web of Science[1] was used to screen studies that presented synthesis processes of silver nanoparticles through chemical and biological reduction, consistently reporting information about the implementation of green chemistry principles. This process – supported by the nanotechnology experts – allowed shaping 8 assessment criteria from the PoVs: type of reducing agent (g_1), type of capping agent (g_2), solvent typology (g_3), use of local resources (g_4), reaction time (g_5) and temperature (g_6), equipment type (g_7) and size range of ensuing nanoparticles (g_8). Table 2 shows their coding together with their preference order, as well as the rationale for their selection. Six criteria are qualitative (g_1–g_4, g_7, g_8) and the two remaining are quantitative (g_5, g_6). In order to install a fair comparison between production protocols, the selection condition was that they had to involve the same type of particles and be usable for the same type of application, which in this case was assumed as being antimicrobial activity.

2.3.1. Structure of the multiple criteria classification method

The rigorous structuring of the problem performed in the previous stages developed a "common language" and understanding between the analysts and the DMs. This proved crucial in understanding the type of MCDA method to be developed, especially considering that the DMs perceived the use of indirect preference elicitation in form of comprehensive judgments on the production processes as their natural way of reasoning. Consequently, indirect preference was assumed as the most relevant elicitation.

Formally, we consider a decision problem involving a finite set of n alternatives, $A = \{a_1, \ldots, a_i, \ldots, a_n\}$, evaluated in terms of m criteria, $G = \{g_1, \ldots, g_j, \ldots, g_m\}$. The performance of a_i on g_j is denoted by $g_j(a_i)$, and the set of all performances on g_j is X_j. To comprehensively measure the implementation of green chemistry principles by the nanoparticles synthesis protocols, we use an additive value function (Keeney & Raiffa, 1976):

$$U(a_i) = \sum_{j=1}^{m} u_j(a_i). \tag{1}$$

Thus, a comprehensive value $U(a_i) \in [0, 1]$ of alternative $a_i \in A$ is derived from the marginal value functions u_j associated with specific criteria. They are used to evaluate the performance of a_i from the specific points of view. Each marginal value function u_j needs to be monotonic, i.e., with the increase of performance, the marginal values are either non-decreasing or non-increasing for, respectively, maximizing (gain-type) or minimizing (cost-type) criteria.

The aim of the study is to assign the nanoparticle synthesis protocols into p preference ordered classes $C_1, \ldots, C_h, \ldots C_p$, such that C_1 and C_p represent, respectively, the worst and the best class. For classification of alternatives, we use a value-driven threshold-based procedure (Greco, Mousseau, & Słowiński, 2010; Zopounidis & Doumpos, 2000) in which the class boundaries are defined with a set of thresholds $\mathbf{b} = \{b_0, \ldots, b_p\}$ on the scale of a comprehensive value, such that $b_{h-1} < b_h$ for $h = 1, \ldots, p$. In this regard,

[1] http://thomsonreuters.com/thomson-reuters-web-of-science/

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

Table 2
Criteria selected for the MCDA assessment of synthesis protocols.

g_j	Criterion	Prefer.	Performance	Enc.	Rationale for the preference order
g_1	Reducing agent class	Gain	Renewable_waste Renewable_primary Synthetic_biodegradable Synthetic	4 3 2 1	The choice of the raw materials plays a pivotal role in affecting the greenness of the synthesis processes. In the reduction of metal ion salts in metal nanoparticles this is implemented by the reducing, capping and solvent types (Ahmad et al., 2010; Baruwati & Varma, 2009; Nadagouda & Varma, 2008a; 2008b) with a possible choice of waste from renewable sources (RW), primary renewable materials (RP), biodegradable polymers (BP) and synthetic chemicals (SC). The selected preference scale was $RW > RP > BP > SC$, with renewable materials as the favorite option because of their non-exhaustible and benign nature. Less preferable choices include the BP, which are generally non-hazardous and lastly synthetic chemicals, commonly hazardous and obtained from laborious dedicated synthesis. The concept of multifunctionality was also included in the capping agent scale, accounting for the fact that some materials can perform the role of both reducing and capping agents (Nadagouda & Varma, 2008b), eliminating the need for a specific capping material. Implementable green chemistry principles: 1, 3, 4, 5, 7, 8, 10, 12 (numbers as used in Table 1).
g_2	Capping agent class	Gain	Not_needed Renewable_waste Renewable_primary Synthetic_biodegradable Synthetic	5 4 3 2 1	
g_3	Solvent class	Gain	Renewable_waste Renewable_primary Synthetic_biodegradable Synthetic	4 3 2 1	
g_4	Local resource use class	Gain	Yes No	1 0	Use of local renewable resources is preferred in comparison with those coming from a distant place, as it has benefits in terms of reduction of transportation impacts and costs. Implementable green chemistry principles: 7.
g_5	Reaction time (seconds)	Cost	Numerical values	–	Shorter reactions (at comparable reaction conditions) imply lower energy consumption, which justifies the need to minimize this criterion. Implementable green chemistry principles: 6, 12.
g_6	Temperature (degrees Celsius)	Cost	Numerical values	–	Ambient (or close to ambient) temperature reactions are preferred as less energy is required and safer operating conditions can be guaranteed when compared to the processes that run at high temperature. Implementable green chemistry principles: 6, 12.
g_7	Equipment type	Gain	Static Stirring_$\leq$ 5 minutes Stirring Micro_sealed_$\leq$ 300 Watts Micro_sealed_$>$ 300 Watts Micro_open Conventional Not_known	8 7 6 5 4 3 2 1	A wide variety of synthesis methods has been advanced for nanosynthesis with static conditions as the preferred option since they do not require any use of energy. Stirring systems are safe and very low energy demanding, thus receiving the second rank (Gill, Appleton, Baganz, & Lye, 2008). Microwave represents an alternative energy source that is preferred to conventional heating as it enhances reaction kinetics by 1–2 orders of magnitude, which can result in shorter reaction times and faster particles formation, as well as reduction in waste production (Gawande et al., 2014; Grace & Pandian, 2007; Komarneni, Li, Newalkar, Katsuki, & Bhalla, 2002; Moseley & Kappe, 2011; Tsuji, Hashimoto, Nishizawa, Kubokawa, & Tsuji, 2005; Varma, 2013; 2014). The worst rank is assigned to lack of reporting on the used equipment, complying with a modeling approach based on worst-case assumption. Implementable green chemistry principles: 1, 6, 11, 12.
g_8	Particles size range	Cost	0–30 nanometers 0–60 nanometers 30–60 nanometers 0–100 nanometers 60–100 nanometers	1 2 3 4 5	The nanoparticles were assumed to be usable for antimicrobial purposes, which implies that the smaller the size the better because their antimicrobial potential is inversely proportional to the size (Duran et al., 2010; Martínez-Castañón, Niño Martínez, Martínez-Gutierrez, Martínez-Mendoza, & Ruiz, 2008; Mohan, Lee, Premkumar, & Geckeler, 2007; Panacek et al., 2006). Ranges, rather than a unique size, were introduced since the synthesis processes normally result in silver nanoparticles that are within boundaries of dimensions.

alternative a_i is assigned to class C_h if $b_{h-1} \leq U(a_i) < b_h$. Moreover, we assume that the comprehensive values of all alternatives are not worse than the lower threshold of the worst class (thus, $b_0 = 0$) and worse than the upper threshold of the best class (thus, $b_p > 1$). The employed procedure is presented graphically in Fig. 2. When using a value-driven threshold-based ordinal classification procedure the preference model is formed by a pair $(U, \mathbf{b})$ consisting of an additive value function U and a vector $\mathbf{b}$ of class thresholds. In this regard, we will call $(U, \mathbf{b})$ a classification model.

An outline of the method we use in the study is given in Fig. 3. It is divided into seven steps (marked as Steps 1–7). By implementing perspectives which are typical for ORDREG (Greco, Kadziński, & Słowiński, 2011; Jacquet-Lagrèze & Siskos, 2001), ROR (Corrente et al., 2013; Greco et al., 2008) and SOR (Kadziński & Tervonen, 2013a; 2013b), these steps provide different views on the certainty of delivered recommendation.

Step 1. In Step 1, we collect the assignment examples for a subset of nanoparticle synthesis protocols $A^R = \{a^*, b^*, \ldots\} \subseteq A$, called reference protocols. The desired assignments are denoted with (Kadziński, Ciomek, and Słowiński (2015a)):

$$a^* \rightarrow [C_{L_{DM}(a^*)}, C_{R_{DM}(a^*)}]. \tag{2}$$

Although, in general, the assignment examples can be imprecise with $L_{DM}(a^*) < R_{DM}(a^*)$, in this study, we will employ precise assignment examples with $L_{DM}(a^*) = R_{DM}(a^*)$. The set of all assignment examples is denoted with *AE*.

Step 2. In Step 2, the method represents the set of provided assignment examples with all pairs $(U, \mathbf{b})$, denoted with $(\mathcal{U}, \mathbf{b})^{AE}$, able to reconstruct *AE*. Each assignment example induces some linear constraints on the parameters of an assumed preference model. Thus, the procedure involves formulation of the following LP model

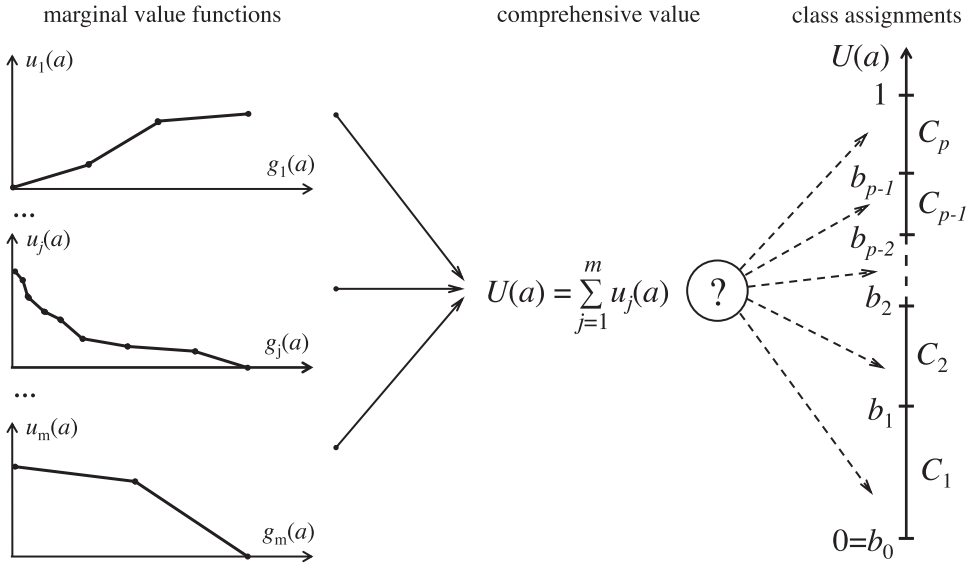

Fig. 2. Value-driven threshold-based multiple criteria ordinal classification.

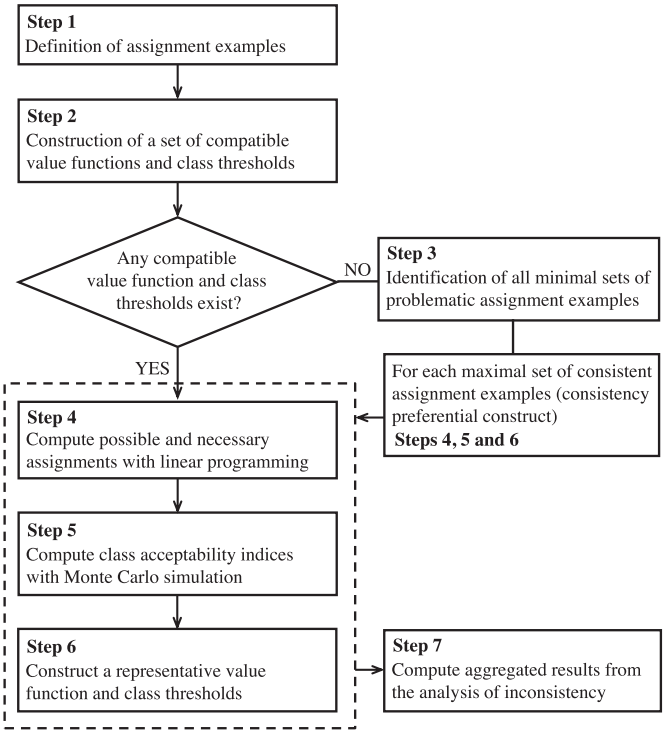

Fig. 3. General outline of the multiple criteria ordinal classification method used in the study.

(Greco et al., 2010):

$$\left.\begin{array}{l} \left.\begin{array}{l} u_j(x_j^k) - u_j(x_j^{k-1}) \geq 0,\ j \in J,\ k = 2, \ldots, n_j(A), \\ u_j(x_j^1) = 0,\ j \in J,\ \sum_{j=1}^{m} u_j(x_j^{n_j(A)}) = 1, \\ b_1 \geq \varepsilon,\ b_{p-1} \leq 1 - \varepsilon, \\ b_h - b_{h-1} \geq \varepsilon,\ h = 2, \ldots, p-1, \end{array}\right\} E^{BASE} \\ \left.\begin{array}{l} U(a^*) \geq b_{L_{DM}(a^*)-1}, \\ U(a^*) + \varepsilon \leq b_{R_{DM}(a^*)}, \end{array}\right\} \forall a^* \in A^R \end{array}\right\} E(AE)$$

where the ordered values of X_j are denoted with $x_j^1, \ldots, x_j^{n_j(A)}$, and $n_j(A) = |X_j|$; $x_j^k < x_j^{k+1}$ for maximizing criteria and $x_j^k > x_j^{k+1}$ for minimizing criteria, $k = 1, \ldots, n_j(A) - 1$.

Note that we use the general marginal value functions with all unique performances corresponding to the characteristic points. In this way, we take advantage only of the ordinal character of performances handling qualitative and quantitative criteria in the same way (Corrente et al., 2013). The set of pairs $(\mathcal{U}, \mathbf{b})^{AE}$ compatible with the provided assignment examples AE is non-empty, if $E(AE)$ is feasible and max ε s.t. $E(AE)$ has an optimal value $\varepsilon^* > 0$. Otherwise, $(\mathcal{U}, \mathbf{b})^{AE}$ is empty.

Step 3. If the set of compatible value functions and class thresholds is empty, we explicitly resolve inconsistency[2]. This requires identification of the minimal subset of troublesome assignment examples which need to be removed to restore consistency. Usually, there exist multiple modifications of the DM's assignment examples leading to preferences representable with an assumed preference model (Mousseau, Dias, & Figueira, 2006). The knowledge of such various way to solve inconsistency is useful for the DM, because it permits him/her to understand the conflicting aspects of the provided assignment examples, understand where and why their statements do not comply with the consistency principle, and to learn about his/her preferences. Traditionally, these different ways for restoring consistency were presented to the DM, who was expected to arbitrarily select a single most desirable one.

In this paper, we propose to analyze all maximal subsets of consistent assignment examples, thus, avoiding an arbitrary selection among different ways to resolve inconsistency. For this purpose, we need to identify all minimal subsets of assignment examples that need to be removed so that the set of compatible pair $(\mathcal{U}, \mathbf{b})$ is non-empty. The procedure starts with solving the following Mixed-Integer Linear Programing (MILP) (Greco et al., 2011; Mousseau et al., 2006):

$$\text{Minimize} f_w = \sum_{a^* \in A^R} v(a^*),\ \text{s.t. } E'(AE), \tag{3}$$

[2] Another option consists in tolerating inconsistency and minimizing the sum of misclassification errors (see Appendix B).

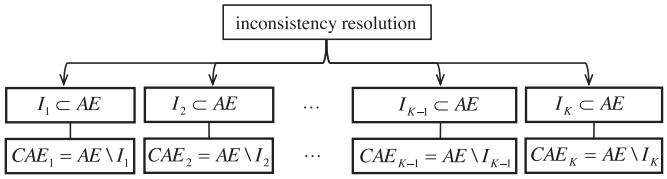

Fig. 4. Multiple ways to resolve inconsistency of the set of assignment examples *AE* with an assumed preference model.

where $E'(AE)$ is defined as follows:

$$\left.\begin{array}{l} E^{BASE}, \\ U(a^*) + v(a^*) \geq b_{L_{DM}(a^*)-1}, \\ U(a^*) + \varepsilon - v(a^*) \leq b_{R_{DM}(a^*)}, \\ v(a^*) \in \{0, 1\}, \end{array}\right\} \forall a^* \in A^R \Bigg\} E'(AE)$$

where w is an index of iteration, because the above procedure will be repeated as many times as there are feasible solutions of problem (3).

This problem indicates a minimal set of constraints that need to be removed from the model constructed in Step 2, so that at least one compatible value function and respective class thresholds can be found. If $v(a^*) = 1$, $a^* \in A^R$ is included in the subset of assignment examples underlying inconsistency. The optimal solution of the above MILP (denoted by *; e.g., f_w^* and $[v^*(a^*),\ a^* \in A^R]$) indicates the first subset of troublesome assignment examples:

$$I_{w=1} = \{a^* \rightarrow [C_{L_{DM}(a^*)}, C_{R_{DM}(a^*)}],\ a^* \in A^R \text{ and } v^*(a^*) = 1\} \subset AE. \tag{4}$$

Let us denote the set of remaining (consistent) assignment examples with $CAE_1 = AE \setminus I_1 \subset AE$. We will call it a consistency preferential construct.

Definition 1. Assuming the use of a particular preference model, a consistency preferential construct for a set of assignment examples *AE* potentially inconsistent with the preference model, is a maximal set of assignment examples in *AE* which can be jointly reproduced by the model. Let us denote it by *CAE*. Consistency construct is maximal in a sense that any of its proper supersets does not allow consistency.

There may exist other subsets of assignment examples underlying inconsistency (see Fig. 4). They can be identified within an iterative procedure (Kadziński, Słowiński, & Greco, 2015b; Mousseau et al., 2006). For this purpose, in each iteration $w = 2, \ldots, K$, we need to solve problem (3) while forbidding finding again the same solutions as found in previous iterations $(w-1, w-2, \ldots, 1)$. This can be achieved by adding the following constraints on the sum of respective binary variables, for $z = 1, \ldots, w-1$:

$$\sum_{a^* \in I_z} v(a^*) \leq f_z^* - 1. \tag{5}$$

Finally, all subsets of assignment examples representing different ways to solve inconsistency are denoted with $I_1, \ldots, I_K$, while the respective consistency preferential constructs with $CAE_1, \ldots, CAE_K$.

Definition 2. Assuming the use of a particular preference model, the consistency preferential core for a set of assignment examples *AE*, is the intersection of all consistency preferential constructs $CAE_1, \ldots, CAE_K$. Let us denote it by $COREAE = \bigcap_{k=1}^{K} CAE_k$.

For the interpretation of preferential reducts, constructs, and cores that refer to the truth or falsity of some robust results rather than analysis of inconsistency, see Kadziński, Corrente, Greco, and Słowiński (2014).

If Step 2 terminates successfully, the method proceeds with Steps 4–6 analyzing the set of value functions and class thresholds compatible with all assignment examples *AE*. Otherwise, these steps are conducted separately for the set of preference models compatible with each CAE_k, $k = 1, \ldots, K$. The logic underlying Steps 4–6 derives from the fact that each compatible model can be applied to assess the alternatives that are not included in the reference set and/or these not contained in the consistency preferential construct.

Step 4. In Step 4, we consider the whole set of compatible models in the spirit of ROR, and compute for each alternative $a_i \in A$ its possible $C_P^{AE}(a_i)$ and necessary $C_N^{AE}(a_i)$ assignments as in UTADIS^{GMS} (Greco et al., 2010). These assignments are supported by, respectively, at least one or all compatible value functions and class thresholds. To verify if $h \in C_P^{AE}(a_i)$, we need to consider the following set of constraints (Kadziński et al., 2015a):

$$\left.\begin{array}{l} U(a_i) \geq b_{h-1}, \text{ if } h \geq 2, \\ U(a_i) + \varepsilon \leq b_h, \text{ if } h \leq p-1, \\ E(AE). \end{array}\right\} E(a_i \rightarrow^P C_h^{AE})$$

If $E(a_i \rightarrow^P C_h^{AE})$ is feasible and $\varepsilon^* > 0$, where $\varepsilon^* = \max\ \varepsilon$ s.t. $E(a_i \rightarrow^P C_h^{AE}) > 0$, then $h \in C_P^{AE}(a_i)$. If the possible assignment is precise, then $C_N^{AE}(a_i) = C_P^{AE}(a_i)$; otherwise, $C_N(a_i) = \emptyset$ (Kadziński & Tervonen, 2013b). Thus defined, $C_P^{AE}(a_i)$ may reflect hesitation with respect to the recommendation suggested by the method for a_i, while $C_N^{AE}(a_i)$ indicates the most certain part of the recommendation unanimously confirmed by all compatible preference models.

Note that if this step was conducted for a consistency construct CAE_k, we would use $E(CAE_k)$ instead of $E(AE)$ in $E(a_i \rightarrow^P C_h^{AE})$. $E(CAE_k)$ involves constraints imposed only by the assignment examples contained in CAE_k. Then, the respective possible and necessary assignments are denoted with $C_P^{CAE_k}(a_i)$ and $C_N^{CAE_k}(a_i)$.

Step 5. In Step 5, we enrich the outcomes of Step 4 with the analysis of probabilities of membership to the particular class. These are materialized with the class acceptability indices $CAI^{AE}(a_i, h) \in [0, 1]$, defined as the share of compatible pairs $(U, \mathbf{t}) \in (\mathcal{U}, \mathbf{t})^{AE}$ that assign alternative a to class C_h (Kadziński & Tervonen, 2013b). Formally, $CAI^{AE}(a_i, h)$ is defined as a multidimensional integral over the space of uniformly distributed value functions and class thresholds compatible with the assignment examples (Kadziński & Tervonen, 2013b):

$$CAI^{AE}(a_i, h) = \int_{(U,\mathbf{b}) \in (\mathcal{U},\mathbf{b})^{AE}} m(U, \mathbf{b}, a_i, h)\, d(U, \mathbf{b}), \tag{6}$$

where $m(U, \mathbf{b}, a_i, h)$ is the class membership function:

$$m(U, \mathbf{b}, a_i, h) = \begin{cases} 1, & \text{if } b_{h-1} \leq U(a_i) < b_h, \\ 0, & \text{otherwise.} \end{cases}$$

To efficiently approximate a value of $CAI^{AE}(a_i, h)$ we apply Monte Carlo simulation as in SOR, and, more specifically, the Hit-And-Run algorithm (Tervonen, van Valkenhoef, Baştürk, & Postmus, 2013). Again, when the analysis is performed for a consistency construct CAE_k, we would consider $(\mathcal{U}, \mathbf{b})^{CAE_k}$ rather than $(\mathcal{U}, \mathbf{b})^{AE}$ and denote the respective outcome by $CAI^{CAE_k}(a_i, h)$.

Step 6. In Step 6, the method constructs a representative value function and class thresholds. Although numerous procedures for selection of such representative model have been proposed in the literature (for a review, see Greco et al., 2011; Beuthe & Scannella, 2001), in this paper we adopt a centroid assignment rule (Angilella, Corrente, & Greco, 2015; Angilella, Corrente, Greco, & Słowiński, 2016; Doumpos, Zopounidis, & Galariotis, 2014). Thus, we construct a representative function U^{AE} as the mean of all models considered

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

in the Monte Carlo simulation performed in Step 5. Formally:

$$u_j^{AE}(a_i) = \sum_{s=1}^{S} u_j^s(a_i)/S \text{ and } b_h^{AE} = \sum_{s=1}^{S} b_h^s/S, \quad (7)$$

where the upper index ^{s} indicates the parameter values observed for the sth model and S is the number of compatible models considered in the simulation. Obviously, since each of these models individually reproduces the assignment examples, the mean model does reproduce them as well. In this way, the representative value function and class thresholds define a central model that can be used for deriving univocal assignment $C_{REP}^{AE}(a_i)$ for each $a_i \in A$ and interpreting the importances of different criteria levels for the classification. The representative results obtained for a consistency construct CAE_k would be denoted by U^{CAE_k} and $C_{REP}^{CAE_k}$.

Step 7. If Step 2 terminated unsuccessfully, the method proceeded with Steps 4–6 for each consistency construct. Then, for CAE_k, $k = 1, \ldots, K$, we computed the possible $C_P^{CAE_k}(a_i)$ and necessary $C_N^{CAE_k}(a_i)$ assignment, the class acceptability indices $CAI^{CAE_k}(a_i, h)$ and the representative value function U^{CAE_k}.

When considering the sets of value functions and class thresholds compatible with all consistency preferential constructs, we can deliver results reflecting two levels of certainty analogously to the case when robustness analysis is conducted for multiple DMs (Greco, Kadziński, Mousseau, & Słowiński, 2012; Kadziński, Słowiński, & Greco, 2016). The first level is related to the necessary (N) or possible (P) consequences of all preference models compatible with each consistency construct, whereas the other refers to the necessary (N) or possible (P) agreement with respect to a set of consistency constructs. This leads to defining four types of assignments:

$$1.\ C_{N,N}^{CAE}(a_i) = \bigcap_{k=1}^{K} C_N^{CAE_k}(a_i), \quad 2.\ C_{N,P}^{CAE}(a_i) = \bigcup_{k=1}^{K} C_N^{CAE_k}(a_i),$$

$$3.\ C_{P,N}^{CAE}(a_i) = \bigcap_{k=1}^{K} C_P^{CAE_k}(a_i), \quad 4.\ C_{P,P}^{CAE}(a_i) = \bigcup_{k=1}^{K} C_P^{CAE_k}(a_i).$$

The most valuable information is provided by $C_{P,N}^{CAE}(a_i)$ and $C_{P,P}^{CAE}(a_i)$. The previous confirms that analysis performed individually for each consistency construct agrees with respect to (some part of) the suggested recommendation, whereas the latter indicates which assignments can be excluded not being confirmed by any compatible model.

With respect to class acceptability indices, a simple idea to aggregate the recommendation obtained for all consistency constructs consists in computing an average value of *CAIs* (Kadziński et al., 2016). Let us call such indicator a cumulative consistency class acceptability index CAI^{CAE}, defined as follows:

$$CAI^{CAE}(a_i, h) = \frac{\sum_{k=1}^{K} CAI^{CAE_k}(a_i, h)}{K}. \quad (8)$$

It reflects the support given to assignment of a_i to class C_h by the sets of preference models compatible with all consistency constructs. Similarly, a preference model U^{CAE} being representative for all consistency constructs can be obtained by averaging the representative models obtained individually for each consistency construct:

$$u_j^{CAE}(a_i) = \sum_{k=1}^{K} u_j^{CAE_k}(a_i)/K \text{ and } b_h^{CAE_k} = \sum_{k=1}^{K} b_h^k/K. \quad (9)$$

Such model is guaranteed to reproduce all assignment examples contained in the consistency preferential core. The assignment it suggests for each $a_i \in A$ is denoted by C_{REP}^{CAE}.

In the proposed approach, the certainty of the recommendation delivered by a single representative classification model is judged in view of robust and stochastic results. This is useful because the recommendation suggested with a single model is not affected by non-uniqueness of compatible sorting models and consistency preferential reducts, at the same time being more precise than the outcomes of ROR and SOR. Thus, the DMs gain confidence in the decision recommendation through the association of a degree of certainty for every classification advanced by the representative model. From another perspective, the possible assignment and class acceptability indices indicate which classes can be excluded, thus minimizing the risk of erroneous decision (Corrente et al., 2013).

3. Construction of the decision recommendation, results and discussion

The final stage of the case study led to the construction of the decision recommendation, i.e., a performance class for nanosynthesis processes based upon their implementation of the principles of green chemistry characterized by the 8 assessment criteria. The set of 53 synthesis protocols was divided into two parts. For 48 reference protocols presented in Table 3, the desired performance class was collected from the two DMs (highly regarded chemists with broad expertise in the area of environmentally friendly nanoparticles synthesis) using a dedicated spreadsheet. The 5 non-reference protocols for which the expert classification was unknown were used to test the decision support provided by the ensuing classification model (see Table 4).

3.1. Identification of DMs' inconsistencies

When using all 48 reference protocols as assignment examples the set of compatible value functions and class thresholds was empty. This indicates inconsistency of assignment examples with an assumed preference model. Inconsistency analysis indicated that there exist three minimal sets of assignment examples that can be removed to restore consistency:

$$I_1 = \{a_{33} \to C_3\}, I_2 = \{a_{12} \to C_1, a_{44} \to C_4\},$$
$$I_3 = \{a_{38} \to C_4, a_{43} \to C_4, a_{48} \to C_5\}. \quad (10)$$

In this regard, let us emphasize that these subsets are minimal in a sense that any of their proper subsets does not resolve inconsistency. In their judgments the experts did not violate the dominance relation, which means that there is no dominated reference protocol assigned to a class better than the dominating one. Thus, the observed inconsistency is likely due to the too limited expressiveness of an assumed additive model which aggregates the performances of each alternative to a single comprehensive value. In any case, the set of classification models is non-empty for the three consistency preferential constructs: $CAE_1 = AE \setminus I_1$, $CAE_2 = AE \setminus I_2$ and $CAE_3 = AE \setminus I_3$, which are composed of 47, 46 and 45 assignment examples, respectively.

3.2. Classification models compatible with each consistency preferential construct

The ORDREG method can operate with every preferential construct and advance a classification model that complies with each of them, thus avoiding the arbitrary choice of modeling paradigm. In Fig. 5 and Table 5, the representative value functions and vectors of class thresholds are presented, respectively.

The character of all representative value functions follows a similar trend for some criteria. In fact, for all three models the shape of marginal value function for the reducing agent (g_1) and reaction time (g_5) is alike and the impact of local resource use (g_4) in the comprehensive value is rather negligible. On the other hand, there are some interesting peculiarities in the models that

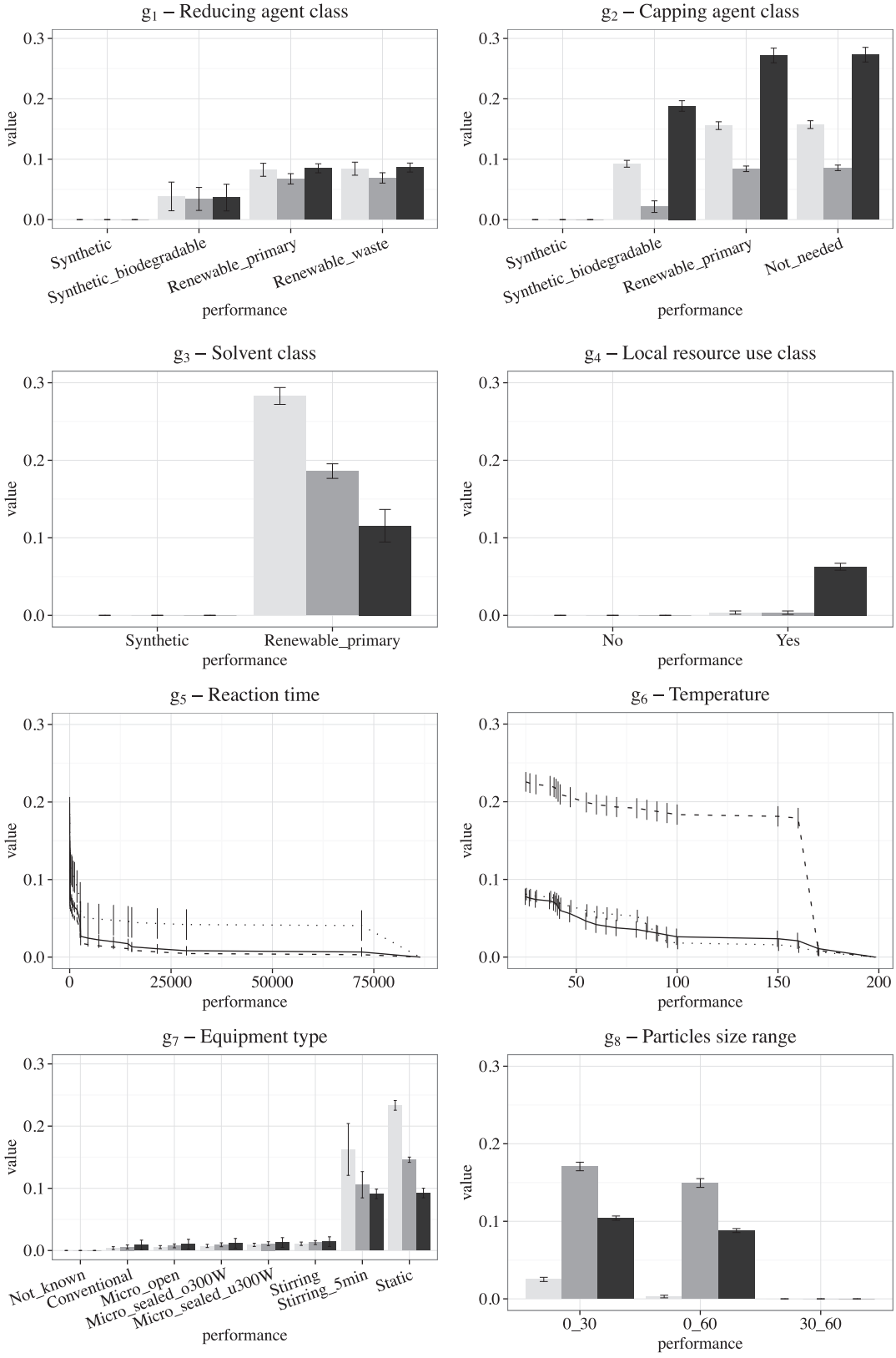

Fig. 5. Representative value functions and distribution of the set of value functions compatible with different consistency preferential constructs ($U_{REP}^{CAE_1}$ – solid line or light gray bars; $U_{REP}^{CAE_2}$ – dashed line or dark gray bars; $U_{REP}^{CAE_3}$ – dotted line or black bars).

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

Table 3
The criteria, performances and desired assignments for the reference nanoparticle synthesis protocols used to construct the preference models (↑ and ↓ indicate maximizing and minimizing criteria, respectively).

	g_1 ↑	g_2 ↑	g_3 ↑	g_4 ↑	g_5 ↓	g_6 ↓	g_7 ↑	g_8 ↓	AE		g_1 ↑	g_2 ↑	g_3 ↑	g_4 ↑	g_5 ↓	g_6 ↓	g_7 ↑	g_8 ↓	AE
a_1	3	2	3	0	45	80.00	3	1	C_3	a_{25}	1	2	3	0	7200	90.00	2	1	C_2
a_2	3	3	3	0	60	100.00	3	1	C_4	a_{26}	1	2	1	0	14,400	160.00	2	3	C_2
a_3	3	3	3	0	72,000	40.00	2	1	C_4	a_{27}	1	2	1	0	14,400	160.00	2	1	C_2
a_4	3	5	3	0	45	41.00	5	1	C_5	a_{28}	3	5	3	0	1800	80.00	2	2	C_4
a_5	3	5	3	0	60	47.00	5	1	C_5	a_{29}	1	5	3	0	480	100.00	4	1	C_2
a_6	3	5	3	0	30	39.00	5	1	C_5	a_{30}	3	3	3	0	7200	70.00	2	1	C_3
a_7	3	5	3	0	30	42.00	5	1	C_5	a_{31}	3	5	3	0	28,800	70.00	2	1	C_3
a_8	3	3	3	0	10	150.00	4	1	C_5	a_{32}	1	1	1	0	60	100.00	3	1	C_2
a_9	1	1	3	0	1800	25.00	6	1	C_2	a_{33}	4	5	3	0	4500	25.00	8	3	C_3
a_{10}	3	1	3	0	900	25.00	1	3	C_2	a_{34}	4	5	3	0	2700	60.00	2	1	C_3
a_{11}	3	1	3	0	900	25.00	1	1	C_2	a_{35}	3	5	3	0	10,800	160.00	2	1	C_3
a_{12}	1	1	1	0	15,300	25.00	6	1	C_1	a_{36}	4	5	3	0	600	40.00	2	1	C_4
a_{13}	3	5	3	0	28,800	25.00	7	2	C_5	a_{37}	3	5	3	0	600	40.00	2	1	C_4
a_{14}	3	5	3	0	28,800	25.00	7	1	C_5	a_{38}	3	5	3	1	900	80.00	2	1	C_4
a_{15}	3	5	3	0	7200	25.00	7	1	C_5	a_{39}	3	5	3	0	600	100.00	4	2	C_4
a_{16}	4	5	3	0	7200	25.00	7	1	C_5	a_{40}	3	5	3	1	1200	100.00	2	1	C_4
a_{17}	3	5	3	1	28,800	37.00	8	1	C_5	a_{41}	3	5	3	0	28,800	25.00	6	2	C_3
a_{18}	3	5	3	1	7200	27.00	8	1	C_5	a_{42}	4	5	3	0	60	55.00	5	1	C_4
a_{19}	3	5	3	1	480	30.00	1	1	C_5	a_{43}	3	5	3	1	600	40.00	2	1	C_4
a_{20}	3	5	3	1	21,600	30.00	8	2	C_5	a_{44}	3	5	3	1	1200	80.00	2	3	C_4
a_{21}	3	5	1	0	86,400	25.00	8	1	C_2	a_{45}	3	5	3	1	900	95.00	2	1	C_4
a_{22}	1	1	1	0	10,800	170.00	4	1	C_1	a_{46}	3	5	3	1	600	25.00	7	1	C_5
a_{23}	1	2	3	0	180	198.00	4	2	C_2	a_{47}	1	1	3	0	60	100.00	4	1	C_2
a_{24}	1	2	3	0	5	100.00	4	1	C_2	a_{48}	3	1	3	0	86,400	25.00	8	1	C_5

Table 4
The performances of non-reference nanoparticle synthesis protocols.

	g_1 ↑	g_2 ↑	g_3 ↑	g_4 ↑	g_5 ↓	g_6 ↓	g_7 ↑	g_8 ↓
a_{49}	3	5	3	0	55	42	5	1
a_{50}	3	2	1	1	2580	85	2	2
a_{51}	2	2	3	0	600	90	2	3
a_{52}	3	3	3	0	70	65	5	1
a_{53}	1	1	1	0	480	100	3	1

Table 5
Representative class thresholds obtained for the analysis of the set of preference models compatible with different consistency preferential constructs.

CAE_k	$b_1^{CAE_k}$	$b_2^{CAE_k}$	$b_3^{CAE_k}$	$b_4^{CAE_k}$
CAE_1	0.131	0.586	0.624	0.696
CAE_2	0.209	0.705	0.733	0.793
CAE_3	0.248	0.643	0.700	0.775

Table 6
Descriptive measures comparing the correlation between comprehensive values and underlying orders of alternatives obtained with different sorting models.

	Pearson correlation coefficient			Kendall's τ		
	CAE_2	CAE_3	Final model	CAE_2	CAE_3	Final model
CAE_1	0.94	0.92	0.98	0.90	0.81	0.91
CAE_2		0.90	0.97		0.81	0.91
CAE_3			0.97			0.87

emerge. For example, differences between the marginal values are significant between relatively medium and good performances for the solvent type (g_3), equipment type (g_7) and particles performance (g_8). In addition, for the capping agent (g_2) and the reaction temperature (g_6), the marginal value functions discriminate strongly also between relatively low performances. The derived models show that for each consistent preferential construct insightful variations for these functions emerge, highlighting slightly different trade-offs between criteria. In particular, for the representative value function obtained for CAE_1, the impact of the solvent class (g_3) and equipment type (g_7) is relatively greater, while the values assigned to the temperature (g_6) and particles' size (g_8) are rather low. On the contrary, the importance of the latter two criteria is higher for the value function obtained for CAE_2, while the representative model constructed for CAE_3 assigns relatively greater importance to the capping agent (g_2).

The analysis of different preference models in compliance with the modeling constraints indicates to the DMs the potential variability of their partial value functions for the assessment criteria. This enriches the learning for DMs on which models represent their preferences and possibly support predilection of certain shapes of criteria value functions rather than others. For example, if capping agent is considered as more relevant, the DM can prefer this underlying model when judging the decision recommendation.

In Appendix A (Table A.12), we present representative comprehensive values and class assignments derived from the analysis of different consistency preferential constructs. Obviously, the values obtained by the same protocol for different models may differ. Nevertheless, the correlation between these scores as well as the underlying orders of alternatives obtained with different models is high (for the values of Pearson correlation coefficient and Kendall's τ, see Table 6). However, it is the comparison of these values with the respective class thresholds that matters and decides upon their classification into one of five pre-defined and ordered classes. Each representative model was able to reproduce the assignment examples contained in the consistency preferential construct (e.g., a_1 is assigned to C_3 as indicated the DM). Overall, all three models assign 42 reference alternatives to the same desired class. The differences concerning reference alternatives underlying inconsistency are summarized in Table 7. Additionally, these protocols are distinguished with a star (*) in the respective columns $C(a_i)$ in Appendix A (Table A.12).

To support interpretation of the representative outcomes, in Fig. 6 we decompose comprehensive values of five exemplary reference protocols into their marginal values and compare them

Table 7
Assignments for the reference alternatives which do not align with the ones desired by the DMs.

Model	Alternative: class desired by the DMs → class imposed by the sorting model
CAE_1	a_{33}: $C_3 \rightarrow C_5$
CAE_2	a_{12}: $C_1 \rightarrow C_2$, a_{44}: $C_4 \rightarrow C_2$
CAE_3	a_{38}: $C_4 \rightarrow C_5$, a_{43}: $C_4 \rightarrow C_5$, a_{48}: $C_5 \rightarrow C_2$
Final model	a_{12}: $C_1 \rightarrow C_2$, a_{33}: $C_3 \rightarrow C_5$, a_{43}: $C_4 \rightarrow C_5$, a_{44}: $C_4 \rightarrow C_2$, a_{48}: $C_5 \rightarrow C_3$

Table 8
The possible assignments, class acceptability indices and representative assignments for the non-reference protocols obtained with the set of preference models compatible with different consistency constructs.

	CAE_1			CAE_2			CAE_3		
	$C_P(a_i)$	$CAI(a_i, h)$	C_{REP}	$C_P(a_i)$	$CAI(a_i, h)$	C_{REP}	$C_P(a_i)$	$CAI(a_i, h)$	C_{REP}
a_{49}	$[C_5, C_5]$	C_5 (1.000)	C_5	$[C_5, C_5]$	C_5 (1.000)	C_5	$[C_5, C_5]$	C_5 (1.000)	C_5
a_{50}	$[C_2, C_2]$	C_2 (1.000)	C_2	$[C_2, C_2]$	C_2 (1.000)	C_2	$[C_2, C_4]$	C_2 (1.000)	C_2
a_{51}	$[C_2, C_3]$	C_2 (1.000)	C_2	$[C_2, C_2]$	C_2 (1.000)	C_2	$[C_2, C_3]$	C_2 (1.000)	C_2
a_{52}	$[C_4, C_4]$	C_4 (1.000)	C_4	$[C_4, C_4]$	C_4 (1.000)	C_4	$[C_4, C_4]$	C_4 (1.000)	C_4
a_{53}	$[C_1, C_2]$	C_1 (0.515) C_2 (0.485)	C_2	$[C_2, C_2]$	C_2 (1.000)	C_2	$[C_1, C_2]$	C_1 (0.888) C_2 (0.112)	C_1

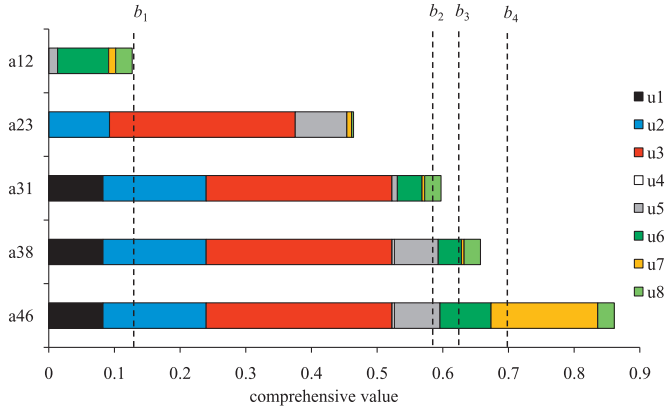

Fig. 6. Marginal and comprehensive values of the five selected reference protocols compared against the representative class thresholds obtained for CAE_1.

against representative class thresholds obtained for CAE_1. This figure clearly illustrates how each criterion contributes to the comprehensive value which, in our study, is interpreted as the overall degree to which different green chemistry principles and quality requirements have been implemented. Importantly, these scores are derived from the joint consideration of all relevant points of view used to build the database. Nevertheless, the decomposition of comprehensive scores into the marginal values exhibits which factors are more decisive in terms of the delivered assignment. The protocols depicted in Fig. 6 represent five different classes. In this way, one can easily see different interpretations of what means comprehensive, considerable, partial, limited and very marginal adoption of green chemistry principles. In particular, all eight criteria vastly contribute to the overall quality for a_{46} being assigned to the best class, while a_{12}, assigned to the worst class, can be considered as relatively good only in terms of temperature (g_6) and particles' size (g_8). Such analysis can be further enhanced by induction of decision rules indicating which levels of marginal values were representative for the alternatives assigned to a given class (or class union). This is illustrated in view of the assignments suggested by the final model in Section 3.3.

When it comes to the classification of non-reference protocols, the three representative models agree with respect to the assignment of a_{49} to C_5, a_{50} and a_{51} to C_2, and a_{52} to C_4 (see Tables 8 and A.12). As for a_{53}, the representative recommendation delivered by the models derived from CAE_1 and CAE_2 is C_2, while the assignment suggested by CAE_3 is C_1. The indications of individual representative classification models can be validated against the outcomes of robust analysis obtained with ROR and SOR (see Table 8). For a_{49} and a_{52}, the possible assignments derived from the analysis of all compatible models are precise, thus, confirming the certainty of recommending C_5 and C_4 for a_{49} and a_{52}, respectively. For a_{50} and a_{51} some compatible models suggest recommendation different from the one delivered with the representative ones. Nevertheless, as indicated by the class acceptability indices, the estimation of probability of an assignment of a_{50} to C_3 or C_4 and a_{51} to C_3 is equal to zero, which means that they are possible only under very specific conditions. Thus, recommendation of an assignment of a_{50} and a_{51} to C_2 can be regarded with certainty. Finally, although preference models CAE_1 and CAE_2 agree with respect to recommending C_2 for a_{53}, the representative class for CAE_3 is C_1. In addition, the class acceptability indices derived from the analysis of CAE_1 and CAE_3 confirm that the share of compatible classification models recommending C_1 is significant, and, thus, needs to be accounted for.

In this perspective, let us add that in Fig. 5, we illustrated the distribution of compatible classification models considered in the Monte Carlo simulation. That is, for each characteristic point apart from the mean marginal value which contributes to the shape of the representative value function, we depicted a standard deviation over 1000 samples used to compute *CAIs*. In this way, we can demonstrate how small is the space of compatible classification models and how well it is represented by the selected mean functions.

3.3. Classification model derived from the analysis of all consistency preferential constructs

The MCDA approach developed for this decision making challenge can also provide a unique classification model that results from the joint consideration of the sets of classification models compatible with all consistency preferential constructs. Fig. 7 illustrates its representative marginal value functions which form an intuitive and easily interpretable output of the applied ORDREG method. It is called the final classification model. Through the use of the general marginal value functions in preference modeling, the method was able to discover non-convex and non-concave classification functions which would not be possible with the classification approaches requiring some pre-defined shape for each per-criterion function (Tervonen, Sepehr, & Kadziński, 2015). This increases transparency and interpretability of the marginal value functions.

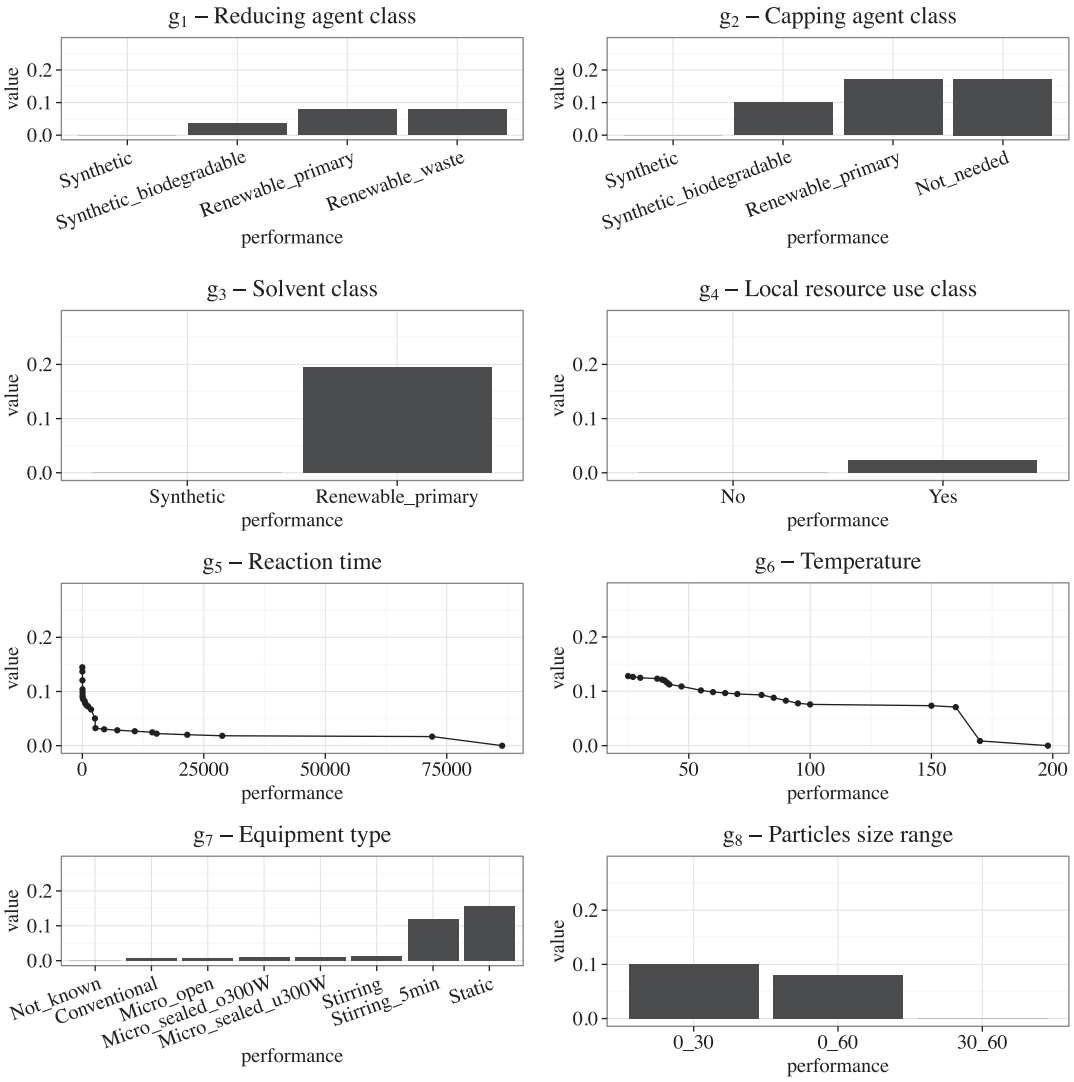

Fig. 7. Representative value function U^{CAE}_{REP} derived from the analysis of preference models compatible with all consistency constructs.

The greatest maximal share in the comprehensive values corresponds to the solvent class (0.195), capping agent (0.172) and equipment type (0.157), while the least maximal share corresponds to local resources use (0.023), reducing agent (0.079) and particles' size (0.100). Thus, although the final classification model indicates that all criteria contribute to the comprehensive score, these maximal shares reflect how big this contribution can be, thus, differentiating the relative importance of different points of view. Similar and complementary results were derived from the application of DRSA on the same dataset (Cinelli et al., 2015).

The variation of marginal values differs significantly from one criterion to another. For the reducing (g_1) and capping (g_2) agents as well as particles' size (g_8), the shapes reflect risk aversion with greater differences between the marginal values observed only for relatively worse performances. For the reaction time (g_5) and equipment type (g_7), the functions' course is risk-seeking with greater marginal values attributed only to the relatively good performances. Finally, the temperature (g_6) has nearly sinusoidal marginal value function shape. The greatest difference of marginal values can be observed for:

- reducing agent (g_1), capping agent (g_2) and solvent class (g_3) when moving from synthetic chemical (1) to biodegradable polymers (2) and primary renewable materials (3);
- reaction time (g_5) when reducing the time to values less than 8 minutes (480 seconds);
- equipment type (g_7) when limiting the use of a stirring plate to at most 5 minutes (i.e., when moving from 6 to 7);
- temperature (g_6) when reducing it from 170 to 160 degrees Celsius.

These transitions indicate the scale ranges where a high value gain in the comprehensive implementation of green chemistry principles can be achieved with limited improvement of evaluation on a particular criterion. On the contrary, the smallest differences of marginal values can be observed for:

- improving upon the use of primary renewable materials (3) on g_1 and g_2;
- equipment type (g_7) ranging from conventional (oil or steam bath; 2) to a stirring plate (6);
- reaction time (g_5) ranging between 480 and 72,000 seconds;
- temperature (g_6) in the range [95, 160].

As a result, improving in these areas does not add much to the overall quality of a protocol.

The comprehensive values and the classification of the nanoparticle protocols obtained with the representative value function U^{CAE}_{REP} are presented in Appendix A (Table A.12). The correlation of the scores and order of alternatives imposed by the final model

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

Table 9
Marginal and comprehensive values of the non-reference protocols with the final classification model.

Protocol	u_1	u_2	u_3	u_4	u_5	u_6	u_7	u_8	$U^{CAE}_{REP}(a_i)$	$C^{CAE}_{REP}(a_i)$
a_{49}	0.078	0.172	0.195	0.000	0.098	0.113	0.011	0.100	0.767	C_5
a_{50}	0.078	0.101	0.000	0.023	0.050	0.088	0.006	0.080	0.427	C_2
a_{51}	0.036	0.101	0.195	0.000	0.078	0.083	0.006	0.000	0.499	C_2
a_{52}	0.078	0.170	0.195	0.000	0.089	0.097	0.011	0.100	0.741	C_4
a_{53}	0.000	0.000	0.000	0.000	0.082	0.076	0.008	0.100	0.266	C_2

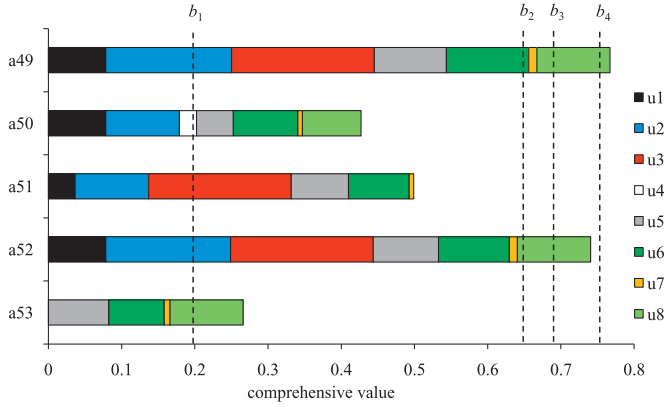

Fig. 8. Marginal and comprehensive values of the non-reference protocols with the final classification model.

with the ones suggested by the models compatible with all consistency preferential constructs is very high (see Table 6). The range of variation of comprehensive values for the protocols assigned to the particular classes is delimited by the following class thresholds:

$$b_1^{CAE} = 0.196,\ b_2^{CAE} = 0.645, b_3^{CAE} = 0.686,\ b_4^{CAE} = 0.754. \quad (11)$$

Since the space of compatible classification models was proven to be rather small, the representative comprehensive values are often close to the class thresholds. In this perspective, it is important to remind that these thresholds are not predefined, but constructed by ORDREG in the same spirit as comprehensive and marginal values. Thus, when discussing the class assignments, the values of protocols and thresholds need to be considered together.

When it comes to the reference protocols, the final model is by definition guaranteed to reproduce classification for the 42 assignment examples contained in the consistency preferential core. The assignment suggested for the misclassified reference alternatives is provided in Table 7.

As for the non-reference protocols, their classification with the final model is provided in Tables 9 and A.12. Its justification is further supported with the decomposition of comprehensive values into the marginal values (see Table 9) and comparing them against respective class thresholds (see Fig. 8).

The assignment of a_{49} to C_5 can be justified by the high consistency with green chemistry principles on all criteria but local resources use (g_4). However, the latter was proven to be the least important one. When compared with a_{49}, a_{52} is slightly worse in terms of capping agent (g_2), reaction time (g_5) and temperature (g_6). This is enough to decrease its status from comprehensive (C_5) to considerable (C_4) adoption of green chemistry principles. Finally, a_{50}, a_{51} and a_{53} are all assigned to C_2, which is interpreted as the limited consistency with the assumed principles. Although a_{50} performs relatively well in terms of reducing (g_1) and capping (g_2) agents, while a_{51} scores positively on capping (g_2) and solvent (g_3) types, they are too weak on the other criteria to be assigned to C_3. Note that when taking into account the range of comprehensive values, C_2 accommodates the greatest variety of protocols. However, for the final classification the distance from the class threshold does not matter. Thus, the implementation of green chemistry principles for all protocols with $U^{CAE}_{REP}(a_i) \in [b_1^{CAE} = 0.198,\ b_2^{CAE} = 0.648)$ is judged as limited. Nevertheless, being close to the upper or lower threshold may indicate greater potential for the improvement or possibility of the degradation, respectively, when the performances of a protocol are slightly changed in the future. What is more, Table 9 highlights the under-performance of the protocols on an individual criterion basis, indicating the parameters that require major attention to increase the overall score. For example, the developers of protocol a_{51} could try to verify whether nanoparticles of smaller and more uniform sizes could be obtained, whereas in case of protocol a_{53} most of the efforts should be firstly directed in producing the nanoparticles through alternative raw materials (e.g., renewable ones) and at lower temperatures.

The recommendation delivered for the non-reference protocols by the final classification model is confirmed by the possible–necessary $C^{P,N}_{CAE}$ and necessary–possible $C^{N,P}_{CAE}$ assignments (see Table 10). The previous indicates that the sets of classification models compatible with all consistency preferential constructs admit such recommendation, while the latter indicates that at least one of these sets confirms it with certainty. Further, the possible–possible assignment $C^{P,P}_{CAE}$ indicates that for a_{49} and a_{52} all other classes than C_5 and C_4, respectively, are excluded as the potential recommendation. For a_{50}, a_{51} and a_{53}, some other classes are possible. However, as indicated by CAI^{CAE} (see Table 10), only for a_{53} the probability of an assignment different from the one delivered by the final model is significant.

To comprehensively explain the recommendation suggested by the final model in terms of the attained marginal values for all alternatives, we use decision rules (Greco, Słowiński, & Zielniewicz, 2013) (see Table 11). Each rule presents the conditions which distinguish a subset of alternatives assigned to a particular class union (e.g., at least class C_4 or at most class C_2) from the remaining ones. The value in the last column of Table 11 indicates how many alternatives supported induction of the respective rule. Overall, rules provide a useful information on the role of particular criteria or their subsets in assigning the alternatives to a given class union. For example, the 4 rules corresponding to the union "at least class C_5" indicate that:

- the alternatives assigned to the best class (C_5) attained some minimal performance thresholds for at least one of the following four pairs of marginal value functions: {u_5, u_7}, {u_1, u_5}, {u_5, u_6} or {u_4, u_6};
- the alternatives in the union "at most class C_4" reached none of these four combinations of marginal performance thresholds.

For illustrative purpose, in Appendix B we report the results obtained with a sorting model minimizing the sum of misclassification errors (Zopounidis & Doumpos, 2000), thus, not explicitly removing inconsistent assignment examples.

4. Conclusions

The performance of sustainability evaluations requires the use of multiple criteria, which normally represent different and

Table 10
Possible assignments for different consistency constructs; the possible–possible, possible–necessary, necessary–possible and necessary–necessary assignments, and cumulative consistency class acceptability indices for the non-reference protocols.

	Possible assignments							
	CAE_1	CAE_2	CAE_3	$C^{P,P}_{CAE}$	$C^{P,N}_{CAE}$	$C^{N,P}_{CAE}$	$C^{N,N}_{CAE}$	CAI^{CAE}
a_{49}	$[C_5, C_5]$	$[C_5, C_5]$	$[C_5, C_5]$	$[C_5, C_5]$	$[C_5, C_5]$	$[C_5, C_5]$	$[C_5, C_5]$	C_5 (1.000)
a_{50}	$[C_2, C_2]$	$[C_2, C_2]$	$[C_2, C_4]$	$[C_2, C_4]$	$[C_2, C_2]$	$[C_2, C_2]$	–	C_2 (1.000)
a_{51}	$[C_2, C_3]$	$[C_2, C_2]$	$[C_2, C_3]$	$[C_2, C_3]$	$[C_2, C_2]$	$[C_2, C_2]$	–	C_2 (1.000)
a_{52}	$[C_4, C_4]$	$[C_4, C_4]$	$[C_4, C_4]$	$[C_4, C_4]$	$[C_4, C_4]$	$[C_4, C_4]$	$[C_4, C_4]$	C_4 (1.000)
a_{53}	$[C_1, C_2]$	$[C_2, C_2]$	$[C_1, C_2]$	$[C_1, C_2]$	$[C_2, C_2]$	$[C_2, C_2]$	–	C_1 (0.468), C_2 (0.532)

Table 11
Decision rules explaining class assignments in terms of marginal values of alternatives.

Decision	Conditions	Support
$Class(a_i) \geq C_5$	$(u_5(a_i) \geq 0.0183)$ and $(u_7(a_i) \geq 0.1197)$	9/17
$Class(a_i) \geq C_5$	$(u_1(a_i) \geq 0.0783)$ and $(u_5(a_i) \geq 0.1208)$	3/17
$Class(a_i) \geq C_5$	$(u_5(a_i) \geq 0.0925)$ and $(u_6(a_i) \geq 0.1090)$	5/17
$Class(a_i) \geq C_5$	$(u_4(a_i) \geq 0.0232)$ and $(u_6(a_i) \geq 0.1200)$	6/17
$Class(a_i) \geq C_4$	$(u_1(a_i) \geq 0.0783)$ and $(u_2(a_i) \geq 0.1705)$ and $(u_5(a_i) \geq 0.0669)$ and $(u_8(a_i) \geq 0.0801)$	19/28
$Class(a_i) \geq C_4$	$(u_2(a_i) \geq 0.1705)$ and $(u_3(a_i) \geq 0.1949)$ and $(u_6(a_i) \geq 0.1200)$ and $(u_8(a_i) \geq 0.1000)$	12/28
$Class(a_i) \geq C_3$	$(u_2(a_i) \geq 0.1705)$ and $(u_5(a_i) \geq 0.0891)$	9/35
$Class(a_i) \geq C_3$	$(u_2(a_i) \geq 0.1705)$ and $(u_3(a_i) \geq 0.1949)$ and $(u_6(a_i) \geq 0.0951)$	25/35
$Class(a_i) \geq C_3$	$(u_1(a_i) \geq 0.0783)$ and $(u_2(a_i) \geq 0.1720)$ and $(u_3(a_i) \geq 0.1949)$ and $(u_8(a_i) \geq 0.0801)$	27/35
$Class(a_i) \geq C_3$	$(u_1(a_i) \geq 0.0783)$ and $(u_5(a_i) \geq 0.1042)$	5/35
$Class(a_i) \geq C_3$	$(u_3(a_i) \geq 0.1949)$ and $(u_7(a_i) \geq 0.1573)$	5/35
$Class(a_i) \geq C_2$	$(u_6(a_i) \geq 0.0710)$	51/52
$Class(a_i) \geq C_2$	$(u_3(a_i) \geq 0.1949)$	45/52
$Class(a_i) \leq C_1$	$(u_2(a_i) \leq 0.0)$ and $(u_6(a_i) \leq 0.0087)$	1/1
$Class(a_i) \leq C_2$	$(u_1(a_i) \leq 0.0)$ and $(u_6(a_i) \leq 0.0710)$	4/18
$Class(a_i) \leq C_2$	$(u_1(a_i) \leq 0.0783)$ and $(u_8(a_i) \leq 0.0)$	4/18
$Class(a_i) \leq C_2$	$(u_3(a_i) \leq 0.0)$ and $(u_5(a_i) \leq 0.0504)$	6/18
$Class(a_i) \leq C_2$	$(u_2(a_i) \leq 0.1006)$ and $(u_7(a_i) \leq 0.0062)$	7/18
$Class(a_i) \leq C_2$	$(u_1(a_i) \leq 0.0)$ and $(u_5(a_i) \leq 0.0669)$	6/18
$Class(a_i) \leq C_3$	$(u_6(a_i) \leq 0.0710)$	5/25
$Class(a_i) \leq C_3$	$(u_2(a_i) \leq 0.1006)$ and $(u_5(a_i) \leq 0.0746)$	10/25
$Class(a_i) \leq C_3$	$(u_5(a_i) \leq 0.0183)$ and $(u_7(a_i) \leq 0.0126)$ and $(u_8(a_i) \leq 0.0801)$	1/25
$Class(a_i) \leq C_3$	$(u_5(a_i) \leq 0.0324)$ and $(u_6(a_i) \leq 0.0987)$	8/25
$Class(a_i) \leq C_4$	$(u_5(a_i) \leq 0.0168)$	3/36
$Class(a_i) \leq C_4$	$(u_5(a_i) \leq 0.0746)$ and $(u_7(a_i) \leq 0.0062)$	16/36
$Class(a_i) \leq C_4$	$(u_4(a_i) \leq 0.0)$ and $(u_7(a_i) \leq 0.0062)$	14/36
$Class(a_i) \leq C_4$	$(u_7(a_i) \leq 0.0126)$ and $(u_8(a_i) \leq 0.0801)$	9/36
$Class(a_i) \leq C_4$	$(u_5(a_i) \leq 0.0669)$ and $(u_7(a_i) \leq 0.0126)$	14/36

somehow conflicting viewpoints. During the last decade materials at the nanoscale, called nanomaterials, have been produced and used increasingly in many sectors to improve the performance of conventional products. However, concerns about the sustainability implications of nanomateirals themselves, as well as their production processes have been raised. The research described in this paper focuses on the latter challenge, proposing a decision aiding approach for assessing the implementation of green chemistry principles by protocols for the synthesis of a common nanomaterial (i.e. silver nanoparticles).

The method starts with collecting from the nanotechnology experts the desired assignments for reference protocols. Then, it resolves inconsistency in thus specified preference information by identifying all maximal subsets of consistent assignments, called consistency preferential constructs. Each construct is represented with a set of preference models composed of an additive value function and class thresholds separating the decision classes. Further, a highly interpretable representative classification model is derived. The recommendation it delivers for the non-reference protocols is validated against the outcomes of robustness analysis. These are materialized with the possible and necessary assignments and class acceptability indices. The final classification model and recommendation are built on the top of indications obtained individually for all consistency preferential constructs.

The proposed method was applied to a real-world case study with 48 reference protocols and 5 non-reference protocols. The constructed models showed that the selected 8 criteria were meaningful for the comprehensive evaluation of the green chemistry principles and played discriminatory roles in the protocol evaluations, even though the initial model could not reproduce all assignment examples. This suggests that some additional evaluation factors, e.g., toxicity of the materials, should be added to the model in case such data is available. However, the method was usable even if the experts' opinion was not fully consistent with an assumed classification model.

The constructed final representative classification model indicated that solvent, capping agent and equipment type have the largest effect on the overall assessment of protocols, while the impact of using local resources is marginal. The use of general value functions allows inferring potentially non-convex and non-concave classification models. This was useful for discovering scale ranges where the improvements of the protocols' performances may bring either high value gains or no gain at all. For example, the character of functions for the reducing and capping agents was risk-averse, whereas for the reaction time or equipment type it was risk-seeking. It means that for these criteria improving an already good performance of the protocol may contribute, respectively, marginally or significantly to its overall evaluation. Such information can be used for prioritizing the different factors when developing new or revising old nanoparticle synthesis protocols.

The proposed method has proven to derive an interpretable classification model for the existing or new protocols. In this case

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

study, it was used to assign the protocols to five pre-defined and ordered classes. When applied to the non-reference protocols, the implementation of green chemistry principles for three out of five considered protocols was judged as limited. For all protocols the decomposition of the comprehensive values into marginal ones indicated which criteria were decisive for the suggested recommendation and in which aspects some quality was missing to attain better classification. The certainty of the delivered recommendation was enhanced with robustness analysis. For four non-reference protocols the suggested assignment was confirmed to be robust, whereas for one protocol the method indicated hesitation between two classes. Such information enables usable decision aiding. The intelligibility of the constructed robust classification model by non-experts in MCDA shows promising potentials of applicability to problems concerning sustainability assessments. Obviously, future research should be oriented towards verification of the constructed model on a more comprehensive set of new protocols.

Overall, this research showed how successful implementation of MCDA in the context of sustainability assessments could be conducted. The MCDA process proved pivotal to structure the problem, leading to co-constructive development by decision analysts and DMs of the alternatives, assessment criteria, problem statement and identification of the appropriate preference elicitation method and the type of model that best satisfied the objective of the case study. Our experiences from developing the method and conducting the case study confirm that a mutual learning of the model, the decision analysts and the DMs is crucial for successful implementation of MCDA approaches to real-world problems.

The study itself demonstrated the usefulness of the proposed method for the evaluation of the "green" claims of nanosynthesis protocols. While the constructed model should not be perceived as a universal tool for green chemistry-based classification of nanoparticles, the approach is promising for developing context-specific classification models for use in similar problems. The desirable properties making the proposed method an appealing solution for decision aiding include:

- accepting indirect preference information in form of assignment examples; in this way, the parameters of a classification model are inferred from the holistic judgments provided by the experts;
- dealing with inconsistency in an automated manner by discovering all minimal sets of conflicting assignment examples;
- handling qualitative and quantitative criteria with general value functions which interpret only the ordinal character of data;
- deriving an easily interpretable numerical score for each alternative by considering jointly all relevant points of view; this allows both better understanding of the suggested recommendation and its confrontation with the experts' expectations and knowledge;
- applying intuitive classification procedure which derives the assignment of alternatives into one of pre-defined and ordered classes from the comparison of alternatives' comprehensive values with the limiting thresholds;
- indicating the level of certainty for the suggested recommendation.

Obviously, the proposed approach is usable in other contexts than nanotechnology. In this perspective, the following limitations need to be considered.

Firstly, when the space of sorting models used to compute the recommendation is large (e.g., in case just few holistic judgments are available), the method might indicate imprecise possible class assignments for some alternatives. Then, the recommendation suggested with a representative model as well as class acceptability indices can be used to stimulate the DM to provide additional assignment examples. Such interactive elicitation of preference information would contract the space of compatible models, thus, increasing the robustness of results obtained with a representative model. In the same spirit, let us emphasize that in case some inconsistency is identified in the provided preference information, the space of models compatible with each consistency construct is usually relatively small, thus, decreasing the variability of possible results.

Secondly, the process of identifying all subsets of assignment examples underlying inconsistency may be computationally demanding (see Section 2.3.1). Therefore, in some cases it may be terminated once, e.g., a desired number of different subsets is obtained or some pre-defined maximal cardinality of an individual subset is reached.

Thirdly, the number of decision rules explaining the suggested class assignments in terms of representative marginal values (see Section 3.3) can be prohibitively large for problems involving numerous alternatives with diverse performance profiles. In this case, one could present to the DM only these rules whose support satisfies some pre-defined threshold (its value can refer to, e.g., the cardinality of a specific class union for which the explanation should be provided). Obviously, one could also generate the rules which incorporate the original performances of alternatives in their condition parts instead of marginal values. In this way, one would provide data-driven explanations as opposed to the model-driven ones presented in this paper.

Finally, let us note that the proposed approach can be adapted to robust multiple criteria ranking (Greco et al., 2008), group decision (Greco et al., 2012; Kadziński et al., 2016) and outranking model (Corrente, Greco, & Słowiński, 2016; Kadziński & Ciomek, 2016). We also envisage implementation of a dedicated decision support system within the *diviz* platform (Meyer & Bigaret, 2012).

Disclaimer

The views expressed in this paper are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency. Any mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Acknowledgments

The authors would like to express their gratitude to Dr. Michael Gonzalez, Dr. David E. Meyer and Dr. Gerardo Ruiz-Mercado from U.S. EPA for their insightful comments during the preparation of the paper, especially on the dataset structure and potential contribution of MCDA in the area of sustainability assessment. The work of Miłosz Kadziński and Krzysztof Ciomek was supported by the Polish Ministry of Science and Higher Education under the Iuventus Plus program in 2016–2019 Grant number IP2015 029674 – 0296/IP2/2016/74. Marco Cinelli, Stuart R. Coles and Kerry Kirwan gratefully acknowledge the funding from the UK Engineering and Physical Sciences Research Council, WMG Department of the University of Warwick (Grant number EP/ K503204/1), the "CL4W", Cleaning Land for Wealth, project (Grant number EP/ K026216/1) and the Innovative Manufacturing Global Research Priority at the University of Warwick (UK). The authors also thank the anonymous reviewers whose remarks helped to improve the paper.

Appendix A. Comprehensive values and class assignment derived with different sorting models considered in the case study

See Table A.12.

Table A.12
Representative comprehensive values and class assignments derived from the analysis of different consistency constructs. Star (*) in column $C(a_i)$ indicates that the recommendation obtained with the model is different than the one desired by the DM.

		CAE_1		CAE_2		CAE_3		Final model				CAE_1		CAE_2		CAE_3		Final model	
a_i	AE	$U(a_i)$	$C(a_i)$	$U(a_i)$	$C(a_i)$	$U(a_i)$	$C(a_i)$	$U^{CAE}_{REP}(a_i)$	$C^{CAE}_{REP}(a_i)$	a_i	AE	$U(a_i)$	$C(a_i)$	$U(a_i)$	$C(a_i)$	$U(a_i)$	$C(a_i)$	$U^{CAE}_{REP}(a_i)$	$C^{CAE}_{REP}(a_i)$
a_1	C_3	0.619	C_3	0.726	C_3	0.692	C_3	0.679	C_3	a_{28}	C_4	0.626	C_4	0.735	C_4	0.714	C_4	0.692	C_4
a_2	C_4	0.665	C_4	0.769	C_4	0.726	C_4	0.720	C_4	a_{29}	C_2	0.573	C_2	0.695	C_2	0.635	C_2	0.634	C_2
a_3	C_4	0.625	C_4	0.734	C_4	0.701	C_4	0.687	C_4	a_{30}	C_3	0.610	C_3	0.722	C_3	0.689	C_3	0.673	C_3
a_4	C_5	0.717	C_5	0.815	C_5	0.798	C_5	0.777	C_5	a_{31}	C_3	0.597	C_3	0.714	C_3	0.683	C_3	0.665	C_3
a_5	C_5	0.699	C_5	0.796	C_5	0.777	C_5	0.758	C_5	a_{32}	C_2	0.144	C_2	0.431	C_2	0.254	C_2	0.276	C_2
a_6	C_5	0.739	C_5	0.833	C_5	0.824	C_5	0.798	C_5	a_{33}	C_3	0.860	C_5*	0.728	C_3	0.699	C_3	0.762	C_5*
a_7	C_5	0.728	C_5	0.823	C_5	0.817	C_5	0.789	C_5	a_{34}	C_3	0.622	C_3	0.732	C_3	0.698	C_3	0.684	C_3
a_8	C_5	0.705	C_5	0.804	C_5	0.782	C_5	0.764	C_5	a_{35}	C_3	0.592	C_3	0.707	C_3	0.647	C_3	0.649	C_3
a_9	C_2	0.458	C_2	0.644	C_2	0.406	C_2	0.503	C_2	a_{36}	C_4	0.692	C_4	0.789	C_4	0.772	C_4	0.751	C_4
a_{10}	C_2	0.510	C_2	0.532	C_2	0.386	C_2	0.476	C_2	a_{37}	C_4	0.690	C_4	0.787	C_4	0.771	C_4	0.749	C_4
a_{11}	C_2	0.535	C_2	0.702	C_2	0.386	C_2	0.476	C_2	a_{38}	C_4	0.657	C_4	0.763	C_4	0.807	C_5*	0.742	C_4
a_{12}	C_1	0.127	C_1	0.418	C_2*	0.244	C_1	0.263	C_2*	a_{39}	C_4	0.629	C_4	0.736	C_4	0.701	C_4	0.689	C_4
a_{13}	C_5	0.774	C_5	0.825	C_5	0.776	C_5	0.791	C_5	a_{40}	C_4	0.645	C_4	0.753	C_4	0.770	C_4	0.723	C_4
a_{14}	C_5	0.796	C_5	0.846	C_5	0.792	C_5	0.811	C_5	a_{41}	C_3	0.622	C_3	0.732	C_3	0.699	C_3	0.684	C_3
a_{15}	C_5	0.810	C_5	0.856	C_5	0.799	C_5	0.722	C_5	a_{42}	C_4	0.692	C_4	0.791	C_4	0.773	C_4	0.752	C_4
a_{16}	C_5	0.812	C_5	0.857	C_5	0.800	C_5	0.823	C_5	a_{43}	C_4	0.693	C_4	0.791	C_4	0.834	C_5*	0.773	C_5*
a_{17}	C_5	0.865	C_5	0.884	C_5	0.852	C_5	0.867	C_5	a_{44}	C_4	0.630	C_4	0.591	C_2*	0.701	C_4	0.689	C_2*
a_{18}	C_5	0.883	C_5	0.898	C_5	0.862	C_5	0.881	C_5	a_{45}	C_4	0.650	C_4	0.757	C_4	0.774	C_4	0.727	C_4
a_{19}	C_5	0.700	C_5	0.796	C_5	0.831	C_5	0.776	C_5	a_{46}	C_5	0.861	C_5	0.900	C_5	0.923	C_5	0.894	C_5
a_{20}	C_5	0.847	C_5	0.867	C_5	0.839	C_5	0.851	C_5	a_{47}	C_2	0.428	C_2	0.619	C_2	0.371	C_2	0.473	C_2
a_{21}	C_2	0.576	C_2	0.695	C_2	0.636	C_2	0.636	C_2	a_{48}	C_5	0.701	C_5	0.796	C_5	0.478	C_2*	0.658	C_3*
a_{22}	C_1	0.063	C_1	0.201	C_1	0.170	C_1	0.145	C_1	a_{49}	–	0.708	C_5	0.805	C_5	0.788	C_5	0.767	C_5
a_{23}	C_2	0.464	C_2	0.429	C_2	0.519	C_2	0.471	C_2	a_{50}	–	0.263	C_2	0.470	C_2	0.549	C_2	0.427	C_2
a_{24}	C_2	0.570	C_2	0.684	C_2	0.622	C_2	0.626	C_2	a_{51}	–	0.518	C_2	0.490	C_2	0.489	C_2	0.499	C_2
a_{25}	C_2	0.457	C_2	0.586	C_2	0.496	C_2	0.513	C_2	a_{52}	–	0.678	C_4	0.780	C_4	0.764	C_4	0.741	C_4
a_{26}	C_2	0.134	C_2	0.217	C_2	0.256	C_2	0.203	C_2	a_{53}	–	0.131	C_2	0.422	C_2	0.245	C_1	0.266	C_2
a_{27}	C_2	0.159	C_2	0.388	C_2	0.361	C_2	0.303	C_2										

Appendix B. Recommendation obtained with the sorting model minimizing the sum of misclassification errors

In this section, we report the results obtained with a sorting model which minimizes the sum of misclassification (overestimation and underestimation) errors (Zopounidis & Doumpos, 2000). When some assignment example cannot be reproduced, such error reflects how much the comprehensive value of the reference alternative would have to be changed so that it is assigned to the class indicated by the DM. Thus, the model tolerates incompatibility, not removing explicitly the inconsistent assignment examples.

For the case study, the minimal sum of misclassification errors was equal to 0.072. The underlying model, denoted with U^{MIN}_{EPS}, misclassified (i.e., assigned to a different class than the one desired by the experts) 7 reference alternatives (a_3 (assigned by the DM to C_4), a_{26} (C_2), a_{28} (C_4), a_{33} (C_3), a_{41} (C_3), a_{42} (C_4) and a_{48} (C_5)). Thus, the number of misclassified protocols is higher than for the models explicitly accounting for the inconsistencies.

The comprehensive values and the classification of the nanoparticle protocols obtained with U^{MIN}_{EPS} are presented in Table B.13, whereas the respective class thresholds are as follows:

$$b^{MIN}_{1,EPS} = 0.035,\ b^{MIN}_{2,EPS} = 0.516,\ b^{MIN}_{3,EPS} = 0.534,\ b^{MIN}_{4,EPS} = 0.549. \tag{B.1}$$

When comparing the comprehensive values computed with U^{MIN}_{EPS} with the ones obtained for other classification models considered in the study, the Kendall's τ and Pearson correlation coefficients are equal to, respectively, 0.87 and 0.80 for $U^{CAE_1}_{REP}$, 0.81 and 0.80 for $U^{CAE_2}_{REP}$, 0.82 and 0.82 for $U^{CAE_3}_{REP}$, and 0.87 and 0.83 for U^{CAE}_{REP}. When it comes to the non-reference alternatives, the recommendation obtained with U^{MIN}_{EPS} is the same as for $U^{CAE_3}_{REP}$, whereas it differs from the assignments suggested by $U^{CAE_1}_{REP}$, $U^{CAE_2}_{REP}$ and U^{CAE}_{REP} only in suggesting that a_{53} should be assigned to C_1 rather than to C_2.

Note that selection of the representative model while minimizing the sum of misclassification errors has some implications on its form. Indeed, the marginal value functions are less discriminative than in case of other models considered in the study. For six criteria the maximal shares in the comprehensive value are not greater than 0.04, whereas clearly higher marginal values (>0.4) are assigned solely to two performances on g_1 and a single performance

Table B.13
Comprehensive values and class assignments obtained with U^{MIN}_{EPS}. Star (*) in column $C(a_i)$ indicates that the recommendation obtained with the model is different than the one desired by the DMs.

a_i	$C(a_i)$	$U(a_i)$	a_i	$C(a_i)$	$U(a_i)$	a_i	$C(a_i)$	$U(a_i)$	a_i	$C(a_i)$	$U(a_i)$	a_i	$C(a_i)$	$U(a_i)$
a_1	C_3	0.533	a_{12}	C_1	0.034	a_{23}	C_2	0.086	a_{34}	C_3	0.529	a_{44}	C_4	0.534
a_2	C_4	0.537	a_{13}	C_5	0.549	a_{24}	C_2	0.515	a_{35}	C_3	0.516	a_{45}	C_4	0.536
a_3	C_3 *	0.524	a_{14}	C_5	0.55	a_{25}	C_2	0.075	a_{36}	C_4	0.546	a_{46}	C_5	0.572
a_4	C_5	0.553	a_{15}	C_5	0.555	a_{26}	C_1 *	0.031	a_{37}	C_4	0.545	a_{47}	C_2	0.07
a_5	C_5	0.549	a_{16}	C_5	0.556	a_{27}	C_2	0.035	a_{38}	C_4	0.539	a_{48}	C_2 *	0.515
a_6	C_5	0.556	a_{17}	C_5	0.551	a_{28}	C_3 *	0.533	a_{39}	C_4	0.534	a_{49}	C_5	0.551
a_7	C_5	0.553	a_{18}	C_5	0.558	a_{29}	C_2	0.101	a_{40}	C_4	0.534	a_{50}	C_2	0.482
a_8	C_5	0.958	a_{19}	C_5	0.551	a_{30}	C_3	0.523	a_{41}	C_4 *	0.534	a_{51}	C_2	0.086
a_9	C_2	0.082	a_{20}	C_5	0.552	a_{31}	C_3	0.519	a_{42}	C_5 *	0.549	a_{52}	C_4	0.544
a_{10}	C_2	0.51	a_{21}	C_2	0.515	a_{32}	C_2	0.035	a_{43}	C_4	0.548	a_{53}	C_1	0.032
a_{11}	C_2	0.514	a_{22}	C_1	0.014	a_{33}	C_5 *	0.554						

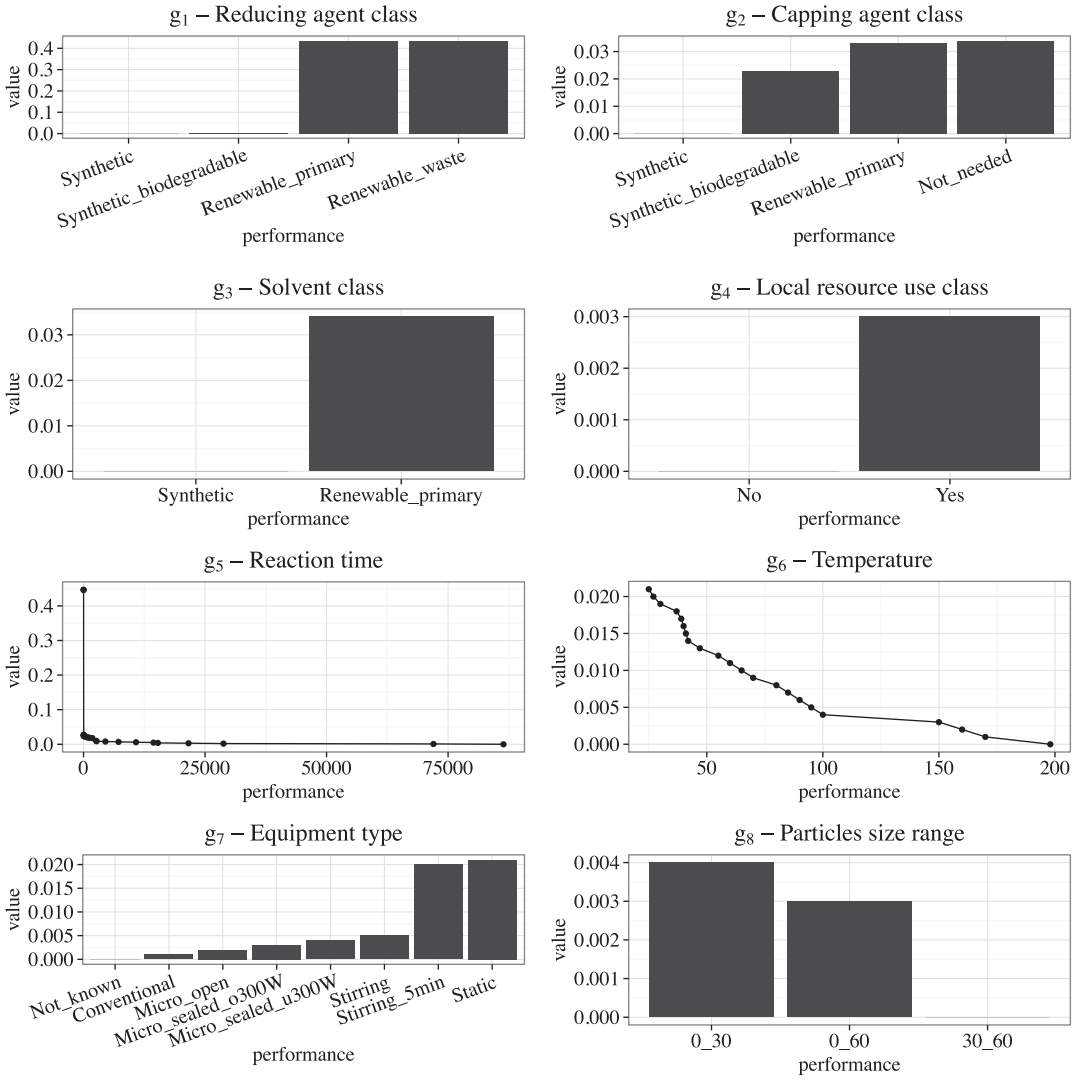

Fig. B.9. Value function U_{EPS}^{MIN} which minimizes the sum of misclassification errors.

on g_5 (see Fig. B.9). Moreover, the ranges of variation of comprehensive values for the alternatives assigned to classes C_1, C_3 and C_4 are very low. In this way, the distances of the misclassified reference alternatives from their desired classes could be lowered. For example, a_{48} is assigned by U_{EPS}^{MIN} to C_2 rather than to C_5, but the misclassification error is just 0.034.

References

Ahmad, N., Sharma, S., Alam, M., Singh, V., Shamsi, S., Mehta, B., et al. (2010). Rapid synthesis of silver nanoparticles using dried medicinal plant of basil. *Colloids and Surfaces B: Biointerfaces, 81*(1), 81–86.

Anastas, P. T., & Warner, J. C. (1998). *Green chemistry: Theory and practice*. New York: Oxford University Press.

Anastas, P. T., & Zimmerman, J. B. (2003). Peer reviewed: Design through the 12 principles of green engineering. *Environmental Science and Technology, 37*, 94A–101A.

Angilella, S., Corrente, S., & Greco, S. (2015). Stochastic multiobjective acceptability analysis for the Choquet integral preference model and the scale construction problem. *European Journal of Operational Research, 240*(1), 172–182.

Angilella, S., Corrente, S., Greco, S., & Słowiński, R. (2016). Robust ordinal regression and stochastic multiobjective acceptability analysis in multiple criteria hierarchy process for the Choquet integral preference model. *Omega, 63*, 154–169.

Baruwati, B., & Varma, R. (2009). High value products from waste: Grape pomace extract – A three-in-one package for the synthesis of metal nanoparticles. *ChemSusChem, 2*(11), 1041–1044.

Bates, M., Larkin, S., Keisler, J., & Linkov, I. (2015). How decision analysis can further nanoinformatics. *Beilstein Journal of Nanotechnology, 6*, 1594–1600.

Bergeson, L. (2013). Sustainable nanomaterials: Emerging governance systems. *ACS Sustainable Chemistry and Engineering, 1*(7), 724–730.

Beuthe, M., & Scannella, G. (2001). Comparative analysis of UTA multicriteria methods. *European Journal of Operational Research, 130*(2), 246–262.

Błaszczyński, J., Słowiński, R., & Szelag, M. (2011). Sequential covering rule induction algorithm for variable consistency rough set approaches. *Information Sciences, 181*(5), 987–1002.

Changseok, H., Andersen, J., Pillai, S., Fagan, R., Falaras, P., Byrne, J., et al. (2013). Green nanotechnology: Development of nanomaterials for environmental and energy applications. In N. Shamim, & V. Sharma (Eds.), *Sustainable nanotechnology and the environment: Advances and achievements* (pp. 201–229). Washington, DC: American Chemical Society. Ch. 14.

Cinelli, M., Coles, S., & Kirwan, K. (2014). Analysis of the potentials of multi criteria decision analysis methods to conduct sustainability assessment. *Ecological Indicators, 46*, 138–148.

Cinelli, M., Coles, S., Nadagouda, M. N., Błaszczyński, J., Słowiński, R., Varma, R. S., et al. (2015). A green chemistry-based classification model for the synthesis of silver nanoparticles. *Green Chemistry, 17*, 2825–2839.

Corrente, S., Greco, S., Kadziński, M., & Słowiński, R. (2013). Robust ordinal regression in preference learning and ranking. *Machine Learning, 93*(2–3), 381–422.

Corrente, S., Greco, S., & Słowiński, R. (2016). Multiple criteria hierarchy process for ELECTRE ri methods. *European Journal of Operational Research, 252*(1), 191–203.

Dahl, J. A., Maddux, B. L. S., & Hutchison, J. E. (2007). Toward greener nanosynthesis. *Chemical Reviews, 107*, 2228–2269.

Das, S., & Marsili, E. (2011). Nanotechnology and sustainability – Current status and future challenges. In M. Rahman (Ed.), *Nanomaterials*. InTech. Ch. 11.

Doumpos, M., & Zopounidis, C. (2011). Preference disaggregation and statistical learning for multicriteria decision support: A review. *European Journal of Operational Research, 209*(3), 203–214.

Doumpos, M., Zopounidis, C., & Galariotis, E. (2014). Inferring robust decision models in multicriteria classification problems: An experimental analysis. *European Journal of Operational Research, 236*(2), 601–611.

Duan, H., Wang, D., & Li, Y. (2015). Green chemistry for nanoparticle synthesis. *Chemical Society Reviews, 44*, 5778–5792.

Dubey, S., Lahtinen, M., & Sillanpaa, M. (2010). Green synthesis and characterizations of silver and gold nanoparticles using leaf extract of Rosa Rugosa. *Colloids and Surfaces A: Physicochemical and Engineering Aspects, 364*(13), 34–41.
Duran, N., Marcato, P., Conti, R. D., Alves, O., Costa, F., & Brocchi, M. (2010). Potential use of silver nanoparticles on pathogenic bacteria, their toxicity and possible mechanisms of action. *Journal of the Brazilian Chemical Society, 21*, 949–959.
Eason, T., Meyer, D., Curran, M., & Upadhyayula, V. (2011). *Guidance to facilitate decisions for sustainable nanotechnology*. Washington, DC: U.S. Environmental Protection Agency.
Eckelman, M. J., Zimmerman, J. B., & Anastas, P. T. (2008). Toward green nano: E–factor analysis of several nanomaterial syntheses. *Journal of Industrial Ecology, 12*, 316–328.
Gawande, M. B., Shelke, S. N., Zboril, R., & Varma, R. S. (2014). Microwave-assisted chemistry: Synthetic applications for rapid assembly of nanomaterials and organics. *Accounts of Chemical Research, 47*, 1338–1348.
Gilbertson, L., Zimmerman, J., Plata, D., Hutchison, J., & Anastas, P. (2015). Designing nanomaterials to maximize performance and minimize undesirable implications guided by the principles of green chemistry. *Chemical Society Reviews, 44*, 5758–5777.
Gill, N., Appleton, M., Baganz, F., & Lye, G. J. (2008). Quantification of power consumption and oxygen transfer characteristics of a stirred miniature bioreactor for predictive fermentation scale-up. *Biotechnology and Bioengineering, 100*, 1144–1155.
Grace, A. N., & Pandian, K. (2007). One pot synthesis of polymer protected Pt, Pd, Ag and Ru nanoparticles and nanoprisms under reflux and microwave mode of heating in glycerol comparative study. *Materials Chemistry and Physics, 104*(1), 191–198.
Greco, S., Kadziński, M., Mousseau, V., & Słowiński, R. (2012). Robust ordinal regression for multiple criteria group decision problems: UTA^{GMS}-GROUP and UTADIS^{GMS}-GROUP. *Decision Support Systems, 52*(3), 549–561.
Greco, S., Kadziński, M., & Słowiński, R. (2011). Selection of a representative value function in robust multiple criteria sorting. *Computers and Operations Research, 38*(11), 1620–1637.
Greco, S., Matarazzo, B., & Słowiński, R. (2001). Rough sets theory for multicriteria decision analysis. *European Journal of Operational Research, 129*, 1–47.
Greco, S., Mousseau, V., & Słowiński, R. (2008). Ordinal regression revisited: Multiple criteria ranking using a set of additive value functions. *European Journal of Operational Research, 191*(2), 415–435.
Greco, S., Mousseau, V., & Słowiński, R. (2010). Multiple criteria sorting with a set of additive value functions. *European Journal of Operational Research, 207*(4), 1455–1470.
Greco, S., Słowiński, R., & Zielniewicz, P. (2013). Putting dominance-based rough set approach and robust ordinal regression together. *Decision Support Systems, 54*(2), 891–903.
Hebbalalu, D., Lalley, J., Nadagouda, M., & Varma, R. (2013). Greener techniques for the synthesis of silver nanoparticles using plant extracts, enzymes, bacteria, biodegradable polymers, and microwaves. *ACS Sustainable Chemistry and Engineering, 1*(7), 703–712.
Hischier, R. (2014). Framework for LCI modelling of releases of manufactured nanomaterials along their life cycle. *The International Journal of Life Cycle Assessment, 19*(4), 838–849.
Hoffman, R., Shadbolt, N., Burton, A., & Klein, G. (1995). Eliciting knowledge from experts: A methodological analysis. *Organizational Behavior and Human Decision Processes, 62*, 129–158.
Hutchison, J. E. (2008). Greener nanoscience: A proactive approach to advancing applications and reducing implications of nanotechnology. *ACS Nano, 2*, 395–402.
Hyeon, T., Manna, L., & Wong, S. (2015). Sustainable nanotechnology. *Chemical Society Reviews, 44*, 5755–5757.
Iavicoli, I., Leso, V., Ricciardi, W., Hodson, L., & Hoover, M. (2014). Opportunities and challenges of nanotechnology in the green economy. *Environmental Health, 13*, 78.
Jacquet-Lagrèze, E., & Siskos, Y. (2001). Preference disaggregation: 20 years of MCDA experience. *European Journal of Operational Research, 130*(2), 233–245.
Kadziński, M., & Ciomek, K. (2016). Integrated framework for preference modeling and robustness analysis for outranking-based multiple criteria sorting with ELECTRE and PROMETHEE. *Information Sciences, 352–353*, 167–187.
Kadziński, M., Ciomek, K., & Słowiński, R. (2015a). Modeling assignment-based pairwise comparisons within integrated framework for value-driven multiple criteria sorting. *European Journal of Operational Research, 241*(3), 830–841.
Kadziński, M., Corrente, S., Greco, S., & Słowiński, R. (2014). Preferential reducts and constructs in robust multiple criteria ranking and sorting. *OR Spectrum, 36*(4), 1021–1053.
Kadziński, M., Słowiński, R., & Greco, S. (2015b). Multiple criteria ranking and choice with all compatible minimal cover sets of decision rules. *Knowledge-Based Systems, 89*, 569–583.
Kadziński, M., Słowiński, R., & Greco, S. (2016). Robustness analysis for decision under uncertainty with rule-based preference model. *Information Sciences, 328*, 321–339.
Kadziński, M., & Tervonen, T. (2013a). Robust multi-criteria ranking with additive value models and holistic pair-wise preference statements. *European Journal of Operational Research, 228*(1), 169–180.
Kadziński, M., & Tervonen, T. (2013b). Stochastic ordinal regression for multiple criteria sorting problems. *Decision Support Systems, 55*(1), 55–66.
Karn, B. (2008). The road to green nanotechnology. *Journal of Industrial Ecology, 12*(3), 263–266.
Karn, B., & Wong, S. (2013). Ten years of green nanotechnology. In N. Shamim, & V. K. Sharma (Eds.), *Sustainable nanotechnology and the environment: Advances and achievements* (pp. 1–10). Washington, DC: American Chemical Society. Ch. 3
Kavitha, K., Syed, B., Rakshith, D., Kavitha, H., Yashwantha, R., Harini, B., et al. (2013). Plants as green source towards synthesis of nanoparticles. *International Research Journal of Biological Sciences, 7*, 66–76.
Kaviya, S., Santhanalakshmi, J., Viswanathan, B., Muthumary, J., & Srinivasan, K. (2011). Biosynthesis of silver nanoparticles using citrus sinensis peel extract and its antibacterial activity. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 79*, 594–598.
Keeney, R., & Raiffa, H. (1976). *Decisions with multiple objectives: Preferences and value trade-offs*. Cambridge: Cambridge University Press.
Komarneni, S., Li, D., Newalkar, B., Katsuki, H., & Bhalla, A. (2002). Microwavepolyol process for Pt and Ag nanoparticles. *Langmuir, 18*(15), 5959–5962.
Korbekandi, H., Iravani, S., & Abbasi, S. (2009). Production of nanoparticles using organisms. *Critical Reviews in Biotechnology, 29*(4), 279–306.
Kou, J., Bennett-Stamper, C., & Varma, R. (2013). Green synthesis of noble nanometals (Au, Pt, Pd) using glycerol under microwave irradiation conditions. *ACS Sustainable Chemistry and Engineering, 1*(7), 810–816.
Kou, J., & Varma, R. (2012). Beet juice utilization: Expeditious green synthesis of noble metal nanoparticles (Ag, Au, Pt, and Pd) using microwaves. *RSC Advances, 2*, 10283–10290.
Linkov, I., Anklam, E., Collier, Z., DiMase, D., & Renn, O. (2014). Risk-based standards: Integrating top–down and bottom–up approaches. *Environment Systems and Decisions, 34*(1), 134–137.
Linkov, I., Kurth, M., Hristozov, D., & Keisler, J. (2015). Nanotechnology: Promoting innovation through analysis and governance. *Environment Systems and Decisions, 35*(1), 22–23.
Linkov, I., & Moberg, E. (2011). *Multi-criteria decision analysis: Environmental applications and case studies*. CRC Press.
Luque, R. (2013). Sustainable nanomaterials: A greener future avenue? *Materials Science and Nanotechnology, 1*, 1–2.
Martínez-Castañón, G. A., Niño Martínez, N., Martínez-Gutierrez, F., Martínez–Mendoza, J. R., & Ruiz, F. (2008). Synthesis and antibacterial activity of silver nanoparticles with different sizes. *Journal of Nanoparticle Research, 10*(8), 1343–1348.
Mata, M., Martins, A., Costa, A., & Sikdar, K. (2015). Nanotechnology and sustainability- Current status and future challenges. In A. Vaseashta (Ed.), *Life cycle analysis of nanoparticles – Risk, assessment, and sustainability* (pp. 271–306). Lancaster, USA: DEStech Publications. Ch. 11
Matus, K. J. M., Hutchinson, J. E., Peoples, R., Rung, S., & Tanguay, R. (2011). *Green nanotechnology challenges and opportunities*. American Chemical Society.
Meyer, D., & Upadhyayula, V. (2014). The use of life cycle tools to support decision making for sustainable nanotechnologies. *Clean Technologies and Environmental Policy, 16*(4), 757–772.
Meyer, P., & Bigaret, S. (2012). Diviz: A software for modeling, processing and sharing algorithmic workflows in MCDA. *Intelligent Decision Technologies, 6*(4), 283–296.
Mohan, Y., Lee, K., Premkumar, T., & Geckeler, K. (2007). Hydrogel networks as nanoreactors: A novel approach to silver nanoparticles for antibacterial applications. *Polymer, 48*(1), 158–164.
Moseley, J., & Kappe, C. (2011). A critical assessment of the greenness and energy efficiency of microwave-assisted organic synthesis. *Green Chemistry, 13*, 794–806.
Mousseau, V., Dias, L., & Figueira, J. (2006). Dealing with inconsistent judgments in multiple criteria sorting models. *4OR, 4*(3), 145–158.
Munda, G. (2005). Multi criteria decision analysis and sustainable development. In J. Figueira, S. Greco, & M. Ehrgott (Eds.), *Multiple criteria decision analysis: State of the art surveys* (pp. 953–986). New York: DEStech Publications, Springer.
Nadagouda, M. N., & Varma, R. S. (2008a). Green synthesis of Ag and Pd nanospheres, nanowires, and nanorods using vitamin B2: Catalytic polymerisation of aniline and pyrrole. *Journal of Nanomaterials*, Article ID782358. doi:10.1155/2008/782358.
Nadagouda, M., & Varma, R. (2008b). Green synthesis of silver and palladium nanoparticles at room temperature using coffee and tea extract. *Green Chemistry, 10*, 859–862.
Nadagouda, M. N., Iyanna, N., Lalley, J., Han, C., Dionysiou, D. D., & Varma, R. S. (2014). Synthesis of silver and gold nanoparticles using antioxidants from blackberry, blueberry, pomegranate and turmeric extracts. *ACS Sustainable Chemistry and Engineering, 2*, 1717–1723.
Naidu, S. (2012). *Towards sustainable development of nanomanufacturing*. University of Tennessee Ph.D. thesis.
Panacek, A., Kvitek, L., Prucek, R., Kolar, M., Vecerova, R., Pizurova, N., et al. (2006). Silver colloid nanoparticles: Synthesis, characterization, and their antibacterial activity. *The Journal of Physical Chemistry B, 110*(33), 16248–16253.
Patete, J. M., Peng, X., Koenigsmann, C., Xu, Y., Karn, B., & Wong, S. S. (2011). Viable methodologies for the synthesis of high-quality nanostructures. *Green Chemistry, 13*, 482–519.
Pati, P., Sean, M., & Vikeseland, P. (2014). Life cycle assessment of green nanoparticle synthesis methods. *Environmental Engineering Science, 31*, 410–420.
Sadik, O., Karn, B., & Keller, A. (2014). Editorial: Sustainable nanotechnology. *ACS Sustainable Chemistry and Engineering, 2*(7), 1543–1544.
Sengul, H., Theis, T., & Ghosh, S. (2008). Toward sustainable nanoproducts. *Journal of Industrial Ecology, 12*(3), 329–359.

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019

Senjen, R. (2009). Challenges and opportunities to green nanotechnologies. *European Environmental Bureau,* Accessed 21.10.2016 at: http://www.bef.lt/fileadmin/Publications/2009-NanoBrochureNo1-WEB_Eng.pdf.

Shapira, P., & Youtie, J. (2012). Background paper 3: The economic contributions of nanotechnology to green and sustainable growth. *OECD and the US National Nanotechnology Initiative,* Accessed 21.10.2016 at: http://www.oecd.org/sti/nano/49932107.pdf.

Shapira, P., & Youtie, J. (2015). The economic contributions of nanotechnology to green and sustainable growth. In V. A. Basiuk, & E. V. Basiuk (Eds.), *Green processes for nanotechnology* (pp. 409–434). Springer International Publishing.

Stark, W., Stoessel, P., Wohlleben, W., & Hafner, A. (2015). Industrial applications of nanoparticles. *Chemical Society Reviews, 44*, 5793–5805.

Subramanian, V., Semenzin, E., Hristozov, D., Zondervan-van den Beuken, E., Linkov, I., & Marcomini, A. (2015). Review of decision analytic tools for sustainable nanotechnology. *Environment Systems and Decisions, 35*(1), 29–41.

Tervonen, T., Sepehr, A., & Kadziński, M. (2015). A multi-criteria inference approach for anti-desertification management. *Journal of Environmental Management, 162*, 9–19.

Tervonen, T., van Valkenhoef, G., Baştürk, N., & Postmus, D. (2013). Hit-and-run enables efficient weight generation for simulation-based multiple criteria decision analysis. *European Journal of Operational Research, 224*(3), 552–559.

Tsang, M., Bates, M., Madison, M., & Linkov, I. (2014). Benefits and risks of emerging technologies: Integrating life cycle assessment and decision analysis to assess lumber treatment alternatives. *Environmental Science and Technology, 48*(19), 11543–11550.

Tsoukiás, A. (2007). On the concept of decision aiding process: An operational perspective. *Annals of Operations Research, 154*(1), 3–27.

Tsuji, M., Hashimoto, M., Nishizawa, Y., Kubokawa, M., & Tsuji, T. (2005). Microwave-assisted synthesis of metallic nanostructures in solution. *Chemistry - A European Journal, 11*(2), 440–452.

Upreti, G., Dhingra, R., Naidu, S., Atuahene, I., & Sawhney, R. (2015). Life cycle assessment of nanomaterials. In *Green processes for nanotechnology: From inorganic to bioinspired nanomaterials* (pp. 393–408). Springer International Publishing.

Varma, R. (2013). Green chemistry with microwave energy. In P. T. Anastas, & J. B. Zimmerman (Eds.), *Innovations in green chemistry and green engineering* (pp. 115–156). New York: Springer.

Varma, R. S. (2014). Journey on greener pathways: From the use of alternate energy inputs and benign reaction media to sustainable applications of nano-catalysts in synthesis and environmental remediation. *Green Chemistry, 16*, 2027–2041.

Virkutyte, J., & Varma, R. S. (2013). Environmentally friendly preparation of metal nanoparticles. In *Sustainable preparation of metal nanoparticles: Methods and applications* (pp. 7–33). The Royal Society of Chemistry.

Zopounidis, C., & Doumpos, M. (2000). PREFDIS: A multicriteria decision support system for sorting decision problems. *Computers and Operations Research, 27*(7–8), 779–797.

Please cite this article as: M. Kadziński et al., Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis, European Journal of Operational Research (2016), http://dx.doi.org/10.1016/j.ejor.2016.10.019